PHY 752 Solid State Physics
11-11:50 AM MWF Olin 107

Plan for Lecture 4:

Reading: Chapter 1 & 2 in MPM;

Continued brief introduction to group theory

1. The "great" orthogonality theorem
2. Character tables
3. Examples

PHY 752 Solid State Physics

MWF 11-11:50 AM	OPL 107	http://www.wfu.edu/~natalie/s15phy752/

Instructor: Natalie Holzwarth	Phone:758-5510	Office:300 OPL	e-mail:natalie@wfu.edu

Course schedule for Spring 2015

(Preliminary schedule -- subject to frequent adjustment.)

	Lecture date	MPM Reading	Topic	Assign.	Due date
1	Mon: 01/12/2015	Chap. 1 & 2	Crystal structures	#1	01/23/2015
2	Wed: 01/14/2015	Chap. 1 & 2	Some group theory	#2	01/23/2015
	Fri: 01/16/2015	No class	NAWH out of town		
	Mon: 01/19/2015	No class	MLK Holiday		
3	Wed: 01/21/2015	Chap. 1 & 2	Some group theory	#3	01/23/2015
4	Mon: 01/23/2015	Chap. 1 & 2	Some more group theory	#4	01/26/2015

Results from last time --
The great orthogonality theorem

Notation: $h \equiv$ order of the group

$R \equiv$ element of the group

$\Gamma^i(R)_{\alpha\beta} \equiv$ ith representation of R

$_{\alpha\beta}$ denote matrix indices

$l_i \equiv$ dimension of the representation

$$\sum_R \left(\Gamma^i(R)_{\mu\nu}\right)^* \Gamma^j(R)_{\alpha\beta} = \frac{h}{l_i}\delta_{ij}\delta_{\mu\alpha}\delta_{\nu\beta}$$

Results from last time -- continued

$$\sum_i l_i^2 = h$$

Character orthogonality theorem:

$$\chi^j(R) \equiv \sum_{\mu=1}^{l_j} \Gamma^j(R)_{\mu\mu}$$

$$\sum_R \left(\chi^i(R)\right)^* \chi^j(R) = h\delta_{ij}$$

Note that all members of the same class have the same character

$$\chi^j(R) \equiv \sum_{\mu=1}^{l_j} \Gamma^j(R)_{\mu\mu}$$

Justification: Suppose that for group elements R, S, and T,
$T = R^{-1}SR$ hence T and S are in the same class.
$\Rightarrow \chi^j(T) = \chi^j(R^{-1}SR) = \chi^j(S)$

Example:

	E	A	B	C	D	F
E	E	A	B	C	D	F
A	A	E	D	F	B	C
B	B	F	E	D	C	A
C	C	D	F	E	A	B
D	D	C	A	B	F	E
F	F	B	C	A	E	D

$$\Gamma^1(A) = \Gamma^1(B) = \Gamma^1(C) = \Gamma^1(D) = \Gamma^1(E) = \Gamma^1(F) = 1$$

$$\Gamma^2(A) = \Gamma^2(B) = \Gamma^2(C) = -1$$

$$\Gamma^2(E) = \Gamma^2(D) = \Gamma^2(F) = 1$$

A two-dimensional representation is

$$\Gamma^3(E) = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \qquad \Gamma^3(A) = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

$$\Gamma^3(B) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix} \quad \Gamma^3(C) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & \frac{1}{2} \end{pmatrix}$$

$$\Gamma^3(D) = \begin{pmatrix} -\frac{1}{2} & \frac{\sqrt{3}}{2} \\ -\frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix} \quad \Gamma^3(F) = \begin{pmatrix} -\frac{1}{2} & -\frac{\sqrt{3}}{2} \\ \frac{\sqrt{3}}{2} & -\frac{1}{2} \end{pmatrix}$$

Character table for this group:

	E	A,B,C	D,F
χ^1	1	1	1
χ^2	1	-1	1
χ^3	2	0	-1

Use of character table for analyzing matrix elements:

Suppose that it is necessary to evaluate a matrix element

$$\langle \Psi_1 | O | \Psi_2 \rangle = \int d^3r \Psi_1^*(\mathbf{r}) O \Psi_2(\mathbf{r})$$

$$= 0 \text{ if } \sum_R \left(\Gamma^i(R)\right)^* \Gamma^j(R) \Gamma^k(R) = 0$$

Matrix element example -- continued

$$\langle \Psi_1 | O | \Psi_2 \rangle = \int d^3r \Psi_1^*(\mathbf{r}) O \Psi_2(\mathbf{r})$$

$$= 0 \text{ if } \sum_R \left(\Gamma^i(R)\right)^* \Gamma^j(R)\Gamma^k(R) = 0$$

$$\text{or } \sum_{\mathcal{e}} N_{\mathcal{e}} \left(\chi^i(\mathcal{e})\right)^* \chi^j(\mathcal{e})\chi^k(\mathcal{e}) = 0$$

Initial state — Operator — Final state

Matrix element example -- continued

	E	A,B,C	D,F
χ^1	1	1	1
χ^2	1	-1	1
χ^3	2	0	-1

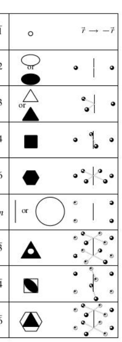
Suppose $O \Rightarrow \chi^2$

Non-trivial matrix elements:

Initial state	$\Rightarrow$	Final state
χ^1	$\Rightarrow$	χ^2
χ^2	$\Rightarrow$	χ^1
χ^3	$\Rightarrow$	χ^3

Some crystal symmetries

Axis type	Schönflies Notation	International Notation	Symbol	Operation
Inversion	$i = S_2$	$\bar{1}$		$\vec{r} \to -\vec{r}$
Twofold	C_2	2	or	
Threefold	C_3	3	or	
Fourfold	C_4	4		
Sixfold	C_6	6		
Twofold Rotoinversion or Mirror	σ_h, $\perp$ to axis; σ_v, plane contains axis; σ_d, bisects twofold axes	$\bar{2} \equiv m$	or	
Threefold Rotoinversion	S_6^{-1}	$\bar{3}$		
Fourfold Rotoinversion	S_4^{-1}	$\bar{4}$		
Sixfold Rotoinversion	S_3^{-1}	$\bar{6}$		



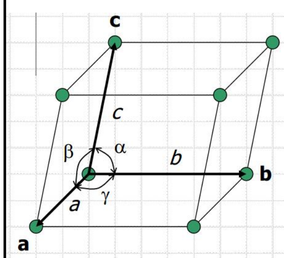
Some crystal symmetries -- cubic symmetry

$$xyz \quad \bar{x}yz \quad x\bar{y}z \quad xy\bar{z} \quad \bar{x}\bar{y}z \quad \bar{x}y\bar{z} \quad x\bar{y}\bar{z} \quad \bar{x}\bar{y}\bar{z}$$
$$yxz \quad \bar{y}xz \quad y\bar{x}z \quad yx\bar{z} \quad \bar{y}\bar{x}z \quad \bar{y}x\bar{z} \quad y\bar{x}\bar{z} \quad \bar{y}\bar{x}\bar{z}$$

..........etc. (48 operations in all)

Point groups -- 32 in all
Space groups (point groups + translations) – 230 in all

Bravais lattice ←→ Reciprocal lattice



(Marder's notation)

$$\mathbf{a}_i \cdot \mathbf{b}_j = 2\pi\delta_{ij}$$

$$\mathbf{b}_i = 2\pi \frac{\mathbf{a}_j \times \mathbf{a}_k}{\left|\mathbf{a}_i \cdot \left(\mathbf{a}_j \times \mathbf{a}_k\right)\right|}$$

Marder's notation

$\mathbf{a} \Rightarrow \mathbf{a}_1$

$\mathbf{b} \Rightarrow \mathbf{a}_2$

$\mathbf{c} \Rightarrow \mathbf{a}_3$

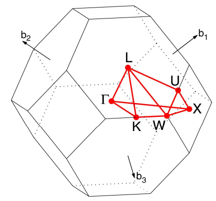
Symmetry associated with wavevector **k**

Electronic wavefunction

$$\Psi_{n\mathbf{k}}(\mathbf{r}+\mathbf{T}) = e^{i\mathbf{k}\cdot\mathbf{T}}\Psi_{n\mathbf{k}}(\mathbf{r})$$

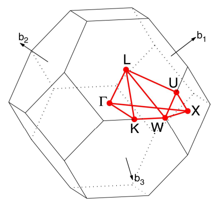
Wigner-Seitz cell of the reciprocal lattice exhibits the symmetry of the wavevectors **k**

Brillouin zone for fcc lattice



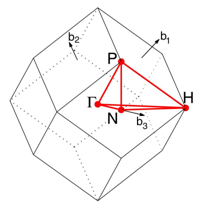
FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]



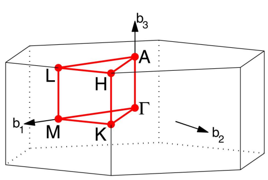
FCC path: Γ-X-W-K-Γ-L-U-W-L-K|U-X

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]



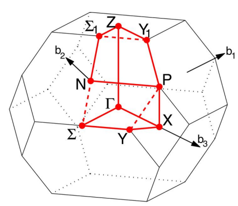
BCC path: Γ-H-N-Γ-P-H|P-N

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]



HEX path: Γ-M-K-Γ-A-L-H-A|L-M|K-H

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]



BCT_2 Path: Γ-X-Y-Σ-Γ-Z-$Σ_1$-N-P-Y_1-Z|X-P

[Setyawan & Curtarolo, DOI: 10.1016/j.commatsci.2010.05.010]

JULY 1, 1936 PHYSICAL REVIEW VOLUME 50

Theory of Brillouin Zones and Symmetry Properties of Wave Functions in Crystals

L. P. Bouckaert,* R. Smoluchowski and E. Wigner, *The Institute for Advanced Study Princeton University, Princeton, New Jersey and the University of Wisconsin*

(Received April 13, 1936)

It is well known that if the interaction between electrons in a metal is neglected, the energy spectrum has a zonal structure. The problem of these "Brillouin zones" is treated here from the point of view of group theory. In this theory, a representation of the symmetry group of the underlying problem is associated with every energy value. The symmetry, in the present case, is the space group, and the main difference as compared with ordinary problems is that while in the latter the representations form a discrete manifold and can be characterized by integers (as e.g., the azimuthal quantum number), the representations of a space group form a continuous manifold, and must be characterized by continuously varying parameters. It can be shown that in the neighborhood of an energy value with a certain representation, there will be energy values with all the representations the parameters of which are close to the parameters of the original representation. This leads to the well-known result that the energy is a continuous function of the reduced wave vector (the components of which are parameters of the above-mentioned kind), but allows in addition to this a systematic treatment of the "sticking" together of Brillouin zones. The treatment is carried out for the simple cubic and the body-centered and face-centered cubic lattices, showing the different possible types of zones.

Brillouin zone for simple cubic lattice

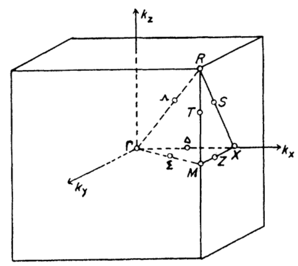


Table I. *Characters of small representations of* Γ, *R*, *H*.

Γ, R, H	E	$3C_4^2$	$6C_4$	$6C_2$	$8C_3$	J	$3JC_4^2$	$6JC_4$	$6JC_2$	$8JC_3$
Γ_1	1	1	1	1	1	1	1	1	1	1
Γ_2	1	1	−1	−1	1	1	1	−1	−1	1
Γ_{12}	2	2	0	0	−1	2	2	0	0	−1
Γ_{15}'	3	−1	1	−1	0	3	−1	1	−1	0
Γ_{25}'	3	−1	−1	1	0	3	−1	−1	1	0
Γ_1'	1	1	1	1	1	−1	−1	−1	−1	−1
Γ_2'	1	1	−1	−1	1	−1	−1	1	1	−1
Γ_{12}'	2	2	0	0	−1	−2	−2	0	0	1
Γ_{15}	3	−1	1	−1	0	−3	1	−1	1	0
Γ_{25}	3	−1	−1	1	0	−3	1	1	−1	0

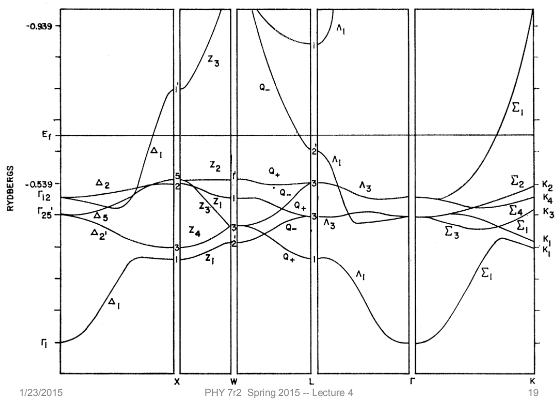
Table II. *Characters for the small representations of* Δ, *T*.

Δ, T	E	C_4^2	$2C_4$	$2JC_4^2$	$2JC_2$
Δ_1	1	1	1	1	1
Δ_2	1	1	−1	1	−1
Δ_2'	1	1	−1	−1	1
Δ_1'	1	1	1	−1	−1
Δ_5	2	−2	0	0	0

Table VII. *Compatibility relations between* Γ *and* Δ, Λ, Σ.

Γ_1	Γ_2	Γ_{12}	Γ_{15}'	Γ_{25}'
Δ_1	Δ_2	$\Delta_1\Delta_2$	$\Delta_1'\Delta_5$	$\Delta_2'\Delta_5$
Λ_1	Λ_2	Λ_3	$\Lambda_2\Lambda_3$	$\Lambda_1\Lambda_3$
Σ_1	Σ_4	$\Sigma_1\Sigma_4$	$\Sigma_2\Sigma_3\Sigma_4$	$\Sigma_1\Sigma_2\Sigma_3$
Γ_1'	Γ_2'	Γ_{12}'	Γ_{15}	Γ_{25}
Δ_1'	Δ_2'	$\Delta_1'\Delta_2'$	$\Delta_1\Delta_5$	$\Delta_2\Delta_5$
Λ_2	Λ_1	Λ_3	$\Lambda_1\Lambda_3$	$\Lambda_2\Lambda_3$
Σ_2	Σ_3	$\Sigma_2\Sigma_3$	$\Sigma_1\Sigma_3\Sigma_4$	$\Sigma_1\Sigma_2\Sigma_4$

Band structure diagram for fcc Cu (Burdick, PR **129** 138-159 (1963))



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