Group Theory

I. Basic mathematical theory with point group and space group examples

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II. Lie groups and their application to particle physics

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Lecture 1

- Definition of a group
- Example of the group of a triangle
- What can group theory do for you?
  - Character Table example
  - Quantum mechanical selection rules
  - Relationships between crystal and atomic / molecular structures

Properties of a Group

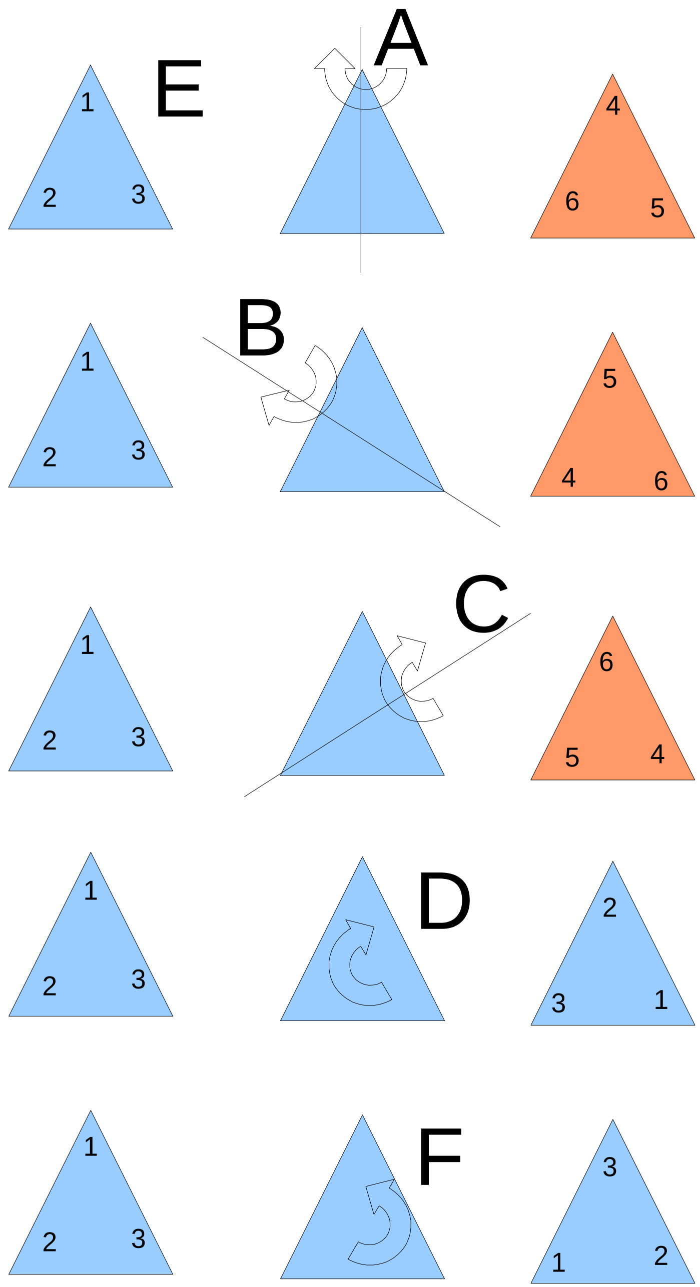
A group is a collection of "elements" – $A, B, C, \ldots$ and a "multiplication" process. The abstract multiplication $(\cdot)$ pairs two group elements, and associates the "result" with a third element. (For example $(A \cdot B = C)$.) The elements and the multiplication process must have the following properties.

1. The collection of elements is closed under multiplication. That is, if elements A and B are in the group and $A \cdot B = C$, element C must be in the group.
2. One of the members of the group is a "unit element" (E). That is, for any element A of the group, $A \cdot E = E \cdot A = A$.
3. For each element A of the group, there is another element A^{-1} which is its "inverse". That is $A \cdot A^{-1} = A^{-1} \cdot A = E$.
4. The multiplication process is "associative". That is for sequential mulplication of group elements A, B, and C, $(A \cdot B) \cdot C = A \cdot (B \cdot C)$.

Group multiplication table

Group of order 6

	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



Example of group theory applied to space groups

Ref: L. P. Bouckaert, R. Smoluchowski, and E. Wigner, *Phys. Rev.* **50**, 58 (1936) – "Theory of Brillouin zones and symmetry properties of wave functions in crystals"

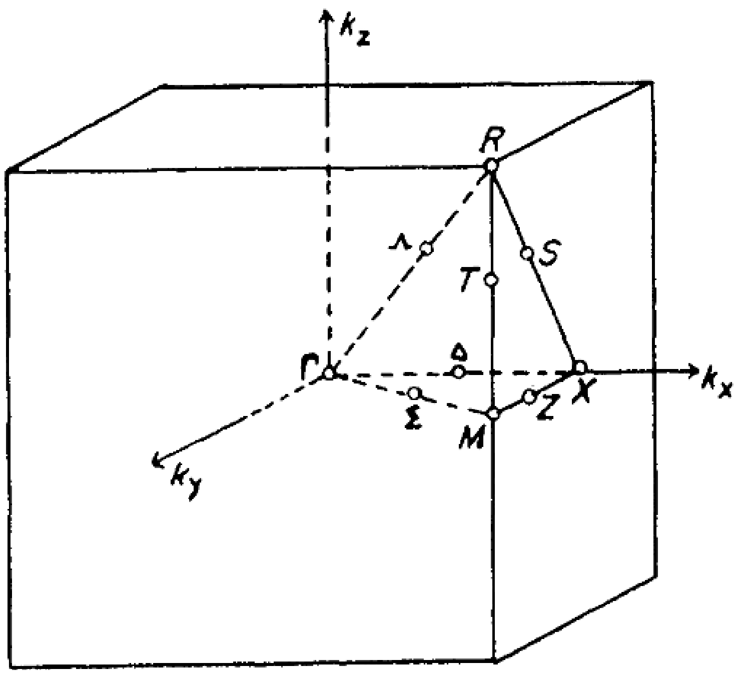
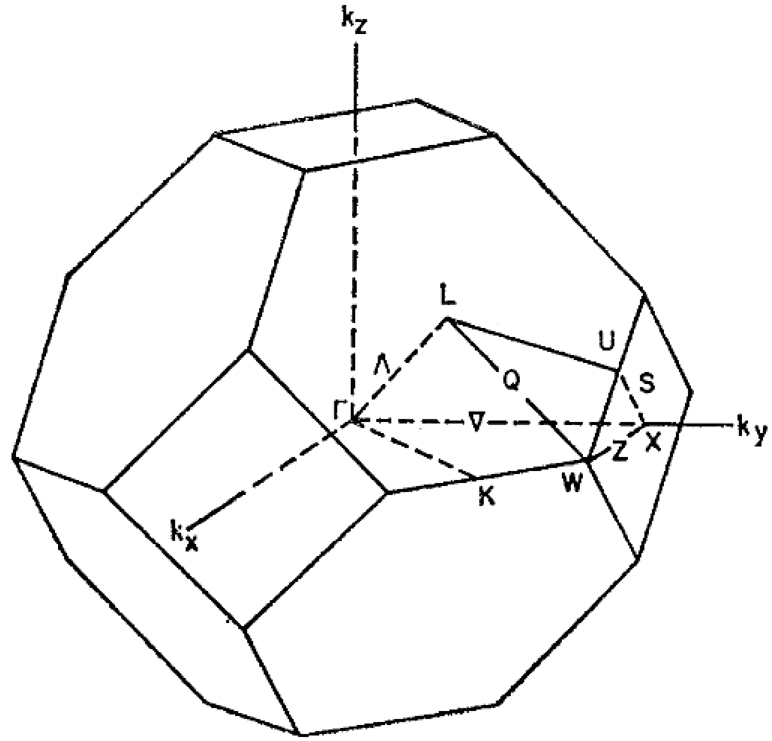


FIG. 2.

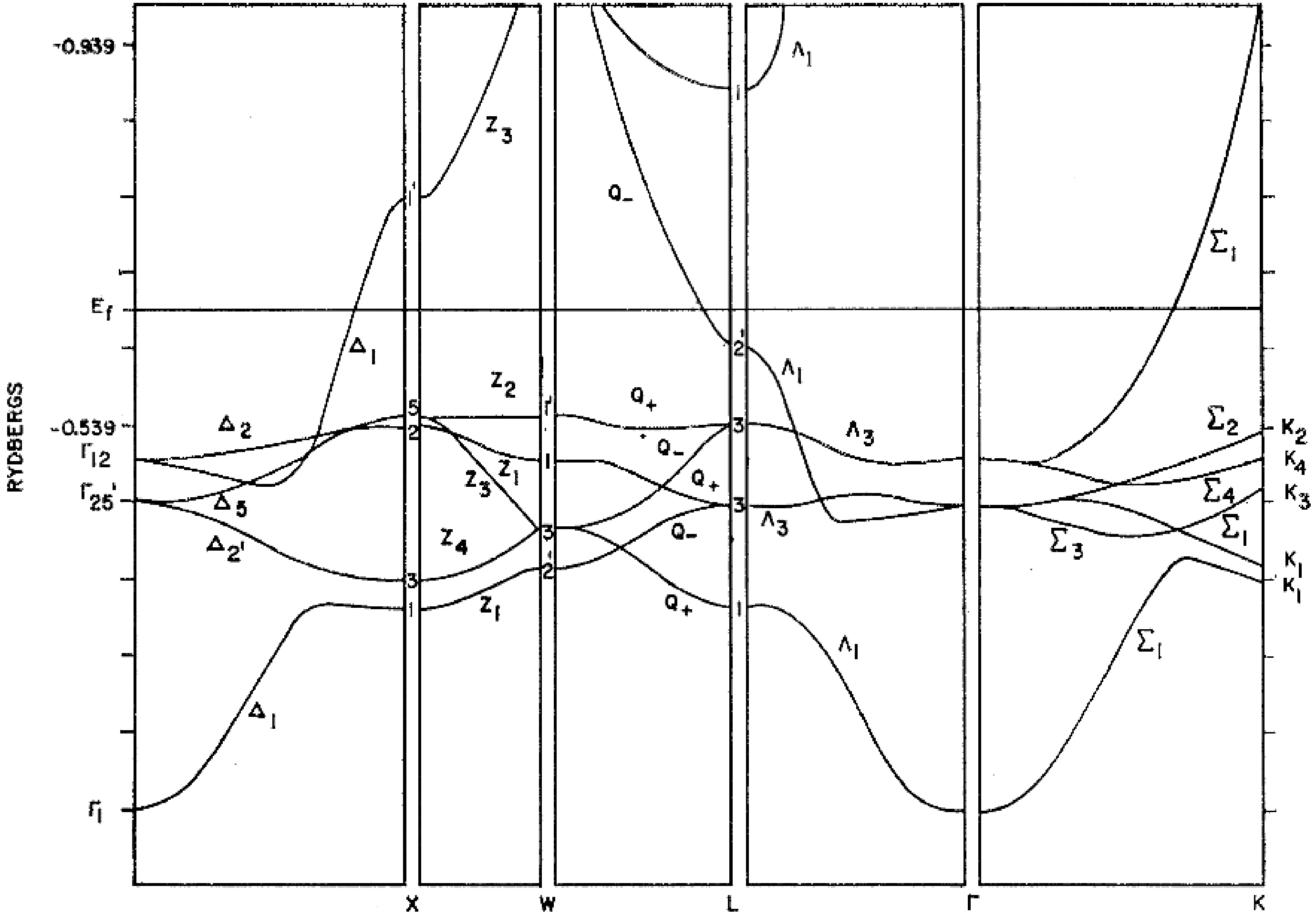
Brillouin zone of simple cubic lattice

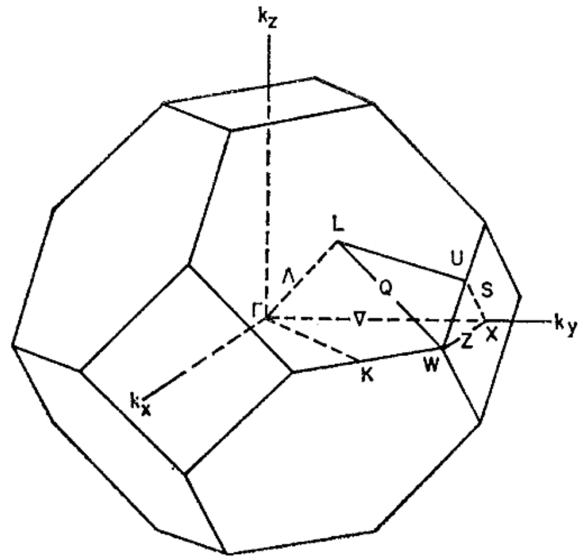


Brillouin zone of face centered cubic lattice

Example of group theory applied to space groups – continued

Ref: G. A. Burdick, *Phys. Rev.* **129**, 138 (1963) – “Energy band structure of copper”





Example of group theory applied to space groups – continued

Ref: BSW – Some appropriate “character tables”

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 V. *Characters of small representations of* M, X.

M X	E E	$2C_4^2$ $2C_4^2\perp$	$C_4^2\perp$ $C_4^2\parallel$	$2C_4\perp$ $2C_4\parallel$	$2C_2$ $2C_2$	J J	$2JC_4^2$ $2JC_4^2\perp$	$JC_4^2\perp$ $JC_4^2\parallel$	$2JC_4\perp$ $2JC_4\parallel$	$2JC_2$ $2JC_2$
M_1	1	1	1	1	1	1	1	1	1	1
M_2	1	1	1	−1	−1	1	1	1	−1	−1
M_3	1	−1	1	−1	1	1	−1	1	−1	1
M_4	1	−1	1	1	−1	1	−1	1	1	−1
M_1'	1	1	1	1	1	−1	−1	−1	−1	−1
M_2'	1	1	1	−1	−1	−1	−1	−1	1	1
M_3'	1	−1	1	−1	1	−1	1	−1	1	−1
M_4'	1	−1	1	1	−1	−1	1	−1	−1	1
M_5	2	0	−2	0	0	2	0	−2	0	0
M_5'	2	0	−2	0	0	−2	0	2	0	0

Example of group theory applied to space groups – continued

Ref: BSW – Some appropriate "compatability tables"

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	$\Sigma_2\Sigma_3$	$\Sigma_1\Sigma_3\Sigma_4$	$\Sigma_1\Sigma_2\Sigma_4$

TABLE IX. *Compatibility relations between X and Δ, Z, S.*

X_1	X_2	X_3	X_4	X_1'	X_2'	X_3'	X_4'	X_5	X_5'
Δ_1	Δ_2	Δ_2'	Δ_1'	Δ_1'	Δ_2'	Δ_2	Δ_1	Δ_5	Δ_5

Example of group theory applied to space groups – continued

Analysis of transitions between quantum mechanical states

$$(\text{Transition probability}) \propto |\mathcal{M}|^2 \equiv \left| \int d^3r \;\; \Psi_f^*(\mathbf{r}) \mathcal{O} \Psi_i(\mathbf{r}) \right|^2 .$$

$$\mathcal{M} \propto \sum_C N_C \chi_f(C) \chi_{\mathcal{O}}(C) \chi_i(C).$$

Some examples:

- Optical transitions (absorption, emission, polarization effects)
- Analysis of phonon modes; Infrared transitions, Raman transitions

Example of group theory applied to point groups

Analysis of "crystal field effects" on atomic states