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

Plan for Lecture 18:

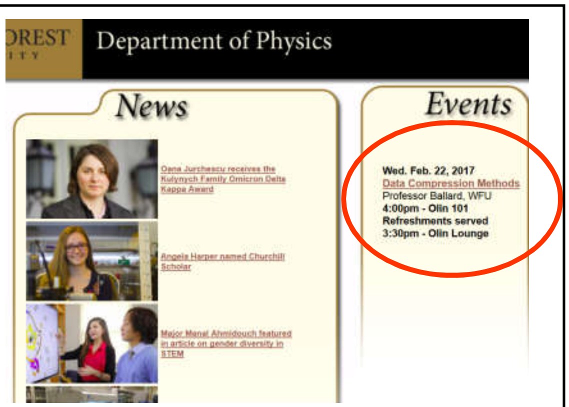
Group theory for the periodic lattice

Reading: Chapter 10 in DDJ

1. **Symmetry of the wave vector**
2. **Compatibility relations**
3. **Symmorphic and non-symmorphic space groups**

This lecture contains some materials from an electronic version of the DDJ text.

9	Wed: 02/01/2017	Chap. 8	Vibrational excitations	#7	02/03/2017
10	Fri: 02/03/2017	Notes	Continuous groups	#8	02/06/2017
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	Chap. 7	Molecular orbital	#13	02/17/2017
16	Fri: 02/17/2017	Chap. 9	Introduction to Space Groups	#14	02/20/2017
17	Mon: 02/20/2017	Chap. 10	Group theory for the periodic lattice		
18	Wed: 02/22/2017	Chap. 10	Group theory for the periodic lattice		
19	Fri: 02/24/2017	Chap. 1-10	Review – Distribute take-home exam		
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				
24	Wed: 03/22/2017				



Space group

Non-lattice translation

$$\{R_\alpha | \boldsymbol{\tau}_\alpha + \mathbf{T}\}$$

Point operation

Lattice translation

Consider the translation subgroup:

$\{\varepsilon|\mathbf{T}\}$

$\mathbf{T} = n_1\mathbf{T}_1 + n_2\mathbf{T}_2 + n_3\mathbf{T}_3$ for all integers n_1, n_2, n_3

$\Rightarrow$ Subgroup is Abelian

$\Rightarrow$ Order of the subgroup is infinite

Reciprocal lattice

Define $\mathbf{G}_i \cdot \mathbf{T}_j = 2\pi\delta_{ij}$

General reciprocal lattice vector:

$$\mathbf{G} = m_1\mathbf{G}_1 + m_2\mathbf{G}_2 + m_3\mathbf{G}_3$$

Effects of point group operations on lattice translations and reciprocal lattice vectors.

Note that $\mathbf{G} \cdot \mathbf{T} = 2\pi N_1$

If R_α is a point operation of the crystal, $R_\alpha\mathbf{T} = \mathbf{T}'$

$\Rightarrow \mathbf{G} \cdot R_\alpha\mathbf{T} = 2\pi N_2 = R_\alpha^{-1}\mathbf{G} \cdot \mathbf{T}$

If R_α point operations act on the translation vectors of the crystal
R_α^{-1} point operations act on the reciprocal lattice vectors

Bloch basis functions

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

Note that $e^{i(\mathbf{k}+\mathbf{G})\cdot\mathbf{T}} = e^{i(\mathbf{k}\cdot\mathbf{T}+M2\pi)} = e^{i\mathbf{k}\cdot\mathbf{T}}$

$\Rightarrow \mathbf{k}$ takes unique values only within the unit cell of the reciprocal lattice

Bloch state $\Psi_{\mathbf{k}}(\mathbf{r})$ is a basis function for the lattice translation subgroup.

Note that $\{R_\alpha|0\}\mathbf{r} = R_\alpha^{-1}\mathbf{r}$

$$\Rightarrow \{R_\alpha|0\} e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot R_\alpha^{-1}\mathbf{r}} u_{\mathbf{k}}(R_\alpha^{-1}\mathbf{r})$$

$$= e^{iR_\alpha\mathbf{k}\cdot\mathbf{r}} u_{R_\alpha\mathbf{k}}(\mathbf{r}) = \Psi_{R_\alpha\mathbf{k}}(\mathbf{r})$$

defining $u_{R_\alpha\mathbf{k}}(\mathbf{r}) \equiv u_{\mathbf{k}}(R_\alpha^{-1}\mathbf{r})$

$$\{\varepsilon|\mathbf{T}\}\{R_\alpha|0\}\Psi_{\mathbf{k}}(\mathbf{r}) = e^{iR_\alpha\mathbf{k}\cdot\mathbf{T}}\Psi_{R_\alpha\mathbf{k}}(\mathbf{r})$$

➔The symmetry of the wavefunction depends on **k**
➔For each **k**, the spatial point symmetries must be considered.

Effects of group operations on Bloch basis functions (symmorphic case)

$$\{R_\alpha|\mathbf{T}\}\Psi_{\mathbf{k}}(\mathbf{r}) = \{\varepsilon|\mathbf{T}\}\{R_\alpha|0\}\Psi_{\mathbf{k}}(\mathbf{r}) = e^{iR_\alpha\mathbf{k}\cdot\mathbf{T}}\Psi_{R_\alpha\mathbf{k}}(\mathbf{r})$$

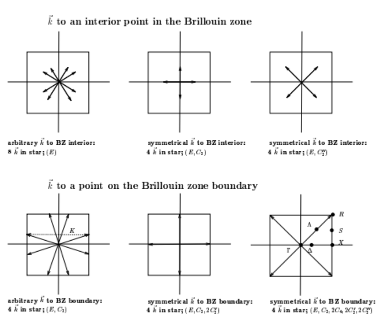
$$= \Psi_{\mathbf{k}}(R_\alpha^{-1}\mathbf{r} + \mathbf{T})$$

If $R_\alpha\mathbf{k} \neq \mathbf{k} + \mathbf{G}$:
the two wavefunctions are not equal but are symmetry related --
$e^{iR_\alpha\mathbf{k}\cdot\mathbf{T}}\Psi_{R_\alpha\mathbf{k}}(\mathbf{r}) = \Psi_{\mathbf{k}}(R_\alpha^{-1}\mathbf{r} + \mathbf{T})$

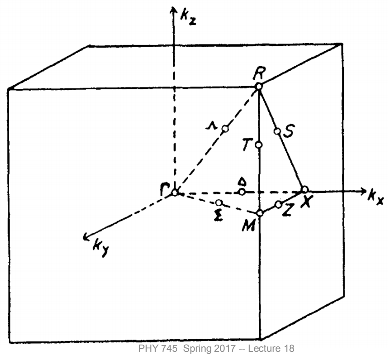
If $R_\alpha\mathbf{k} = \mathbf{k} + \mathbf{G}$:
R_α is an operation in the group of wavevector **k**

Definition: The group of the wave vector is formed by the set of operations which transform **k**➔**k+G**, where **G** is any reciprocal lattice vector.

Example D_4

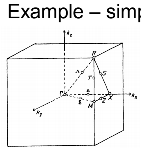


Unit cells of reciprocal space – Brillouin zones
→simple cubic lattice



Definition: The group of the wave vector is formed by the set of operations which transform **k**→**k+G**, where **G** is any reciprocal lattice vector.

Example – simple cubic lattice



For $\mathbf{k}=0$ (Γ) group of the wave vector is full O_h point symmetry

For $\mathbf{k}=k_x\hat{\mathbf{x}}$ $0<k_x<\frac{\pi}{a}$ (Δ) group of the wave vector has C_{4v} symmetry

k=0 in a cubic crystal

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

Γ

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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

Δ

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

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	$\rightarrow\Delta_1$
Γ_2	1	1	−1	−1	1	1	1	−1	−1	1	$\rightarrow\Delta_2$
Γ_{12}	2	2	0	0	−1	2	2	0	0	−1	$\rightarrow\Delta_1\Delta_2$
Γ_{15}'	3	−1	1	−1	0	3	−1	1	−1	0	$\rightarrow\Delta_1'\ \Delta_5$
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	

Compatability relations computed by BSW:

Γ_1	Γ_2	Γ_{12}	Γ_{15}'	Γ_{25}'
Δ_1	Δ_2	$\Delta_1\Delta_2$	$\Delta_1'\Delta_5$	$\Delta_2'\Delta_5$
Γ_1'	Γ_2'	Γ_{12}'	Γ_{15}	Γ_{25}
Δ_1'	Δ_2'	$\Delta_1'\Delta_2'$	$\Delta_1\Delta_5$	$\Delta_2\Delta_5$

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