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

Plan for Lecture 17:

Group theory for the periodic lattice

Reading: Chapter 10 in DDJ

1. **Bloch Theorem and reciprocal space**
2. **Group theory for reciprocal space**
3. **Examples**

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

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

Lattice translation

Point operation

Consider the translation subgroup:

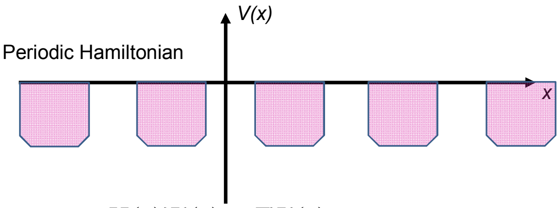
$$\{\varepsilon | \mathbf{T}\}$$

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

$\Rightarrow$ Subgroup is Abelian

$\Rightarrow$ Order of the subgroup is infinite

Periodic Hamiltonian



$$H(\mathbf{r})\Psi(\mathbf{r}) = E\Psi(\mathbf{r})$$
$$H(\mathbf{r}+\mathbf{T})\Psi(\mathbf{r}+\mathbf{T}) = E\Psi(\mathbf{r}+\mathbf{T})$$
$$H(\mathbf{r})\Psi(\mathbf{r}+\mathbf{T}) = E\Psi(\mathbf{r}+\mathbf{T})$$
$$\Rightarrow \Psi(\mathbf{r}+\mathbf{T}) = C\Psi(\mathbf{r})$$
$$\Rightarrow C = e^{i\theta}$$

Accounting for distinct values of $C = e^{i\theta}$

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

Reciprocal lattice

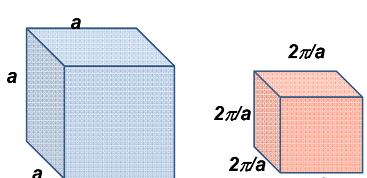
Define $\mathbf{G}_i \cdot \mathbf{T}_j = 2\pi\delta_{ij}$

General reciprocal lattice vector:

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

Example

Simple cubic lattice in real space:



$\mathbf{T}_1 = a\hat{\mathbf{x}}$ $\quad \mathbf{G}_1 = \frac{2\pi}{a}\hat{\mathbf{x}}$

$\mathbf{T}_2 = a\hat{\mathbf{y}}$ $\quad \mathbf{G}_2 = \frac{2\pi}{a}\hat{\mathbf{y}}$

$\mathbf{T}_3 = a\hat{\mathbf{z}}$ $\quad \mathbf{G}_3 = \frac{2\pi}{a}\hat{\mathbf{z}}$

Accounting for distinct values of $C = e^{i\theta}$

$$\theta = \mathbf{k} \cdot \mathbf{T}$$

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

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.

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

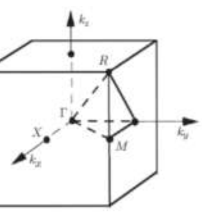


Figure 2.17 Brillouin zone for the simple cubic lattice. Some high symmetry points are indicated: $\Gamma = 0$; $X = (2\pi/a)(1/2, 0, 0)$; $M = (2\pi/a)(1/2, 1/2, 0)$; $R = (2\pi/a)(1/2, 1/2, 1/2)$.

Unit cells of reciprocal space – Brillouin zones
➔face-centered cubic lattice

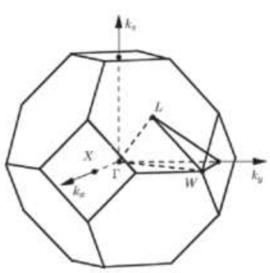


Figure 2.18 Brillouin zone for the face-centered cubic lattice (truncated octahedron). Some high symmetry points are: $\Gamma = 0$; $X = (2\pi/a)(1, 0, 0)$; $L = (2\pi/a)(1/2, 1/2, 1/2)$; $W = (2\pi/a)(1/2, 1, 0)$.

Unit cells of reciprocal space – Brillouin zones
➔body-centered cubic lattice

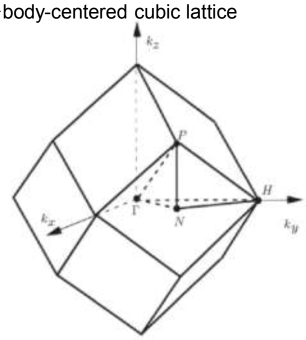


Figure 2.19 Brillouin zone for the body-centered cubic lattice (rhombic dodecahedron). Some high symmetry points are also indicated: $\Gamma = 0$; $N = (2\pi/a)(1/2, 1/2, 0)$; $P = (2\pi/a)(1/2, 1/2, 1/2)$; $H = (2\pi/a)(0, 1, 0)$.

Unit cells of reciprocal space – Brillouin zones
➔hexagonal lattice

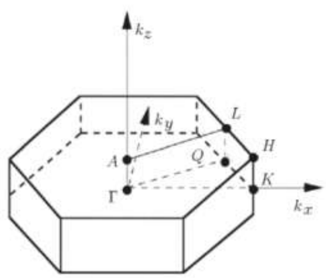


Figure 2.20 Brillouin zone for the hexagonal Bravais lattice. Some high symmetry points are also indicated: $\Gamma = 0$; $K = (2\pi/a)(2/3, 0, 0)$; $Q = (\pi/a)(1, 1/\sqrt{3}, 0)$; $A = (\pi/c)(0, 0, 1)$.

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

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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.

Effects of space group operations on Bloch functions

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

$$\Rightarrow \Psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}}u_{\mathbf{k}}(\mathbf{r})$$

$$\text{where } u_{\mathbf{k}}(\mathbf{r}+\mathbf{T}) = u_{\mathbf{k}}(\mathbf{r})$$

General space group element: $\{R_\alpha | \boldsymbol{\tau}_\alpha + \mathbf{T}\}$

First consider symorphic case where $\boldsymbol{\tau}_\alpha = 0$:

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

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

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

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

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

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

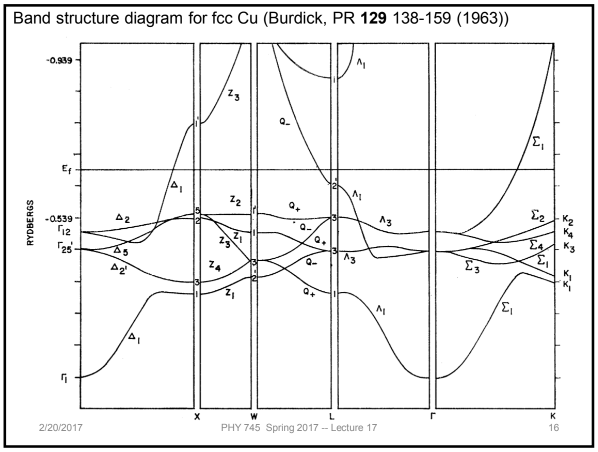
$$\{\varepsilon|\mathbf{T}\}\{R_\alpha|0\}\Psi_{\mathbf{k}}(\mathbf{r}) = e^{iR_\alpha\mathbf{k}\cdot\mathbf{T}}\Psi_{R_\alpha\mathbf{k}}(\mathbf{r})$$

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

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


Band structure diagram for fcc Cu (Burdick, PR 129 138-159 (1963))
RYDBERGS
-0.939
-0.539
X
W
L
Γ
K
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