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

Plan for Lecture 20:

Space group properties

Chapter 10 in DDJ

1. **Non-symmorphic space groups**
2. **Example -- diamond**

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	Chap. 10	Space group representations		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				
25	Fri: 03/24/2017				

Space group

Non-lattice translation

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

Point operation

Lattice translation

Bloch basis functions

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

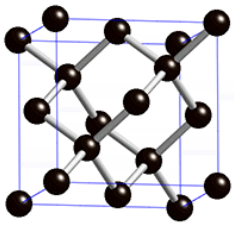
Effects of group operations on Bloch basis functions (symmorphic case)

$$\{R_\alpha|\mathbf{T}\}\Psi_{\mathbf{k}}(\mathbf{r}) = \{\varepsilon|\mathbf{T}\}\{R_\alpha|0\}\Psi_{\mathbf{k}}(\mathbf{r}) = e^{iR_\alpha\mathbf{k}\cdot\mathbf{T}}\Psi_{R_\alpha\mathbf{k}}(\mathbf{r})$$
$$= \Psi_{\mathbf{k}}(R_\alpha^{-1}\mathbf{r}+\mathbf{T})$$

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 $\mathbf{k}$

Non-symmorphic space group
Example -- diamond



https://en.wikipedia.org/wiki/Diamond_cubic

Space group symmetry of diamond

$Fd\bar{3}m$ (#227)
$\Rightarrow$ 24 elements with $\tau_\alpha = 0$
$\Rightarrow$ 24 elements with $\tau_\alpha = \frac{1}{4}(\hat{\mathbf{x}}+\hat{\mathbf{y}}+\hat{\mathbf{z}}) \equiv \tau_d$
10 classes for point symmetry:

$\{E\|0\}$	$\{i\|\tau_d\}$
$8\{C_3\|0\}$	$8\{iC_3\|\tau_d\}$
$3\{C_2\|0\}$	$3\{iC_2\|\tau_d\}$
$6\{iC_2'\|0\}$	$6\{C_2'\|\tau_d\}$
$6\{iC_4\|0\}$	$4\{C_2\|\tau_d\}$

➔Maps to O_h point symmetry

From BSW paper Phys. Rev. **50**, 58 (1936)

TABLE I. *Characters of small representations of* Γ

Γ	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

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

$$\left\{R_\alpha \middle| \tau_\alpha + \mathbf{T}\right\}\Psi_{\mathbf{k}}(\mathbf{r}) = \left\{\varepsilon \middle| \tau_\alpha + \mathbf{T}\right\}\left\{R_\alpha \middle| 0\right\}\Psi_{\mathbf{k}}(\mathbf{r}) = e^{iR_\alpha \mathbf{k}\cdot(\tau_\alpha+\mathbf{T})}\Psi_{R_\alpha \mathbf{k}}(\mathbf{r})$$
$$= \Psi_{\mathbf{k}}(R_\alpha^{-1}\mathbf{r} + \tau_\alpha + \mathbf{T})$$

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 $\mathbf{k}$

Example: Δ direction : $\mathbf{k} = \frac{2\pi\kappa}{a}\hat{\mathbf{x}}$

Character table for C_{4v} symmetry representing Δ

k-point in diamond structure in terms of phase factor $f \equiv e^{i\pi\kappa/2}$

	$\{E\|0\}$	$\{C_4^2\|0\}$	$2\{C_4\|\tau_d\}$	$2\{iC_4^2\|\tau_d\}$	$2\{iC_2'\|0\}$
Δ_1	1	1	f	f	1
Δ_2	1	1	$-f$	f	-1
$\Delta_{2'}$	1	1	$-f$	$-f$	1
$\Delta_{1'}$	1	1	f	$-f$	-1
Δ_5	2	-2	0	0	0

From BSW paper Phys. Rev. **50**, 58 (1936)

Δ_1	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

BAND STRUCTURE AND OPTICAL PROPERTIES OF DIAMOND*

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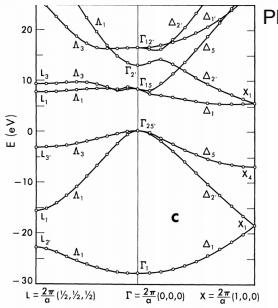

FIG. 1. The electronic band structure of diamond.

PRL **16**, 354 (1966)