Group Applications to Band Theory

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Group Theory, Spring 2015

Outline

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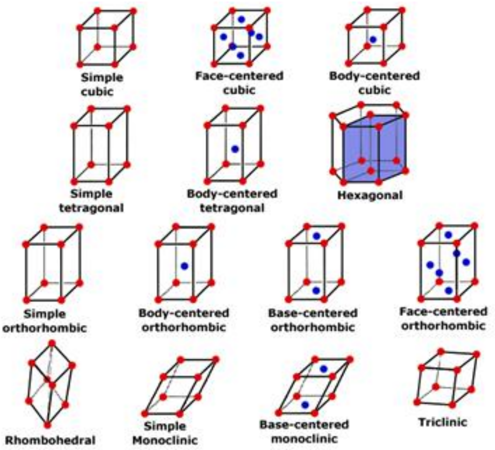
Space Groups

- Crystals are characterized by space groups
- Symmetry under translations and point group operations
- 73 total symmorphic (simple) space groups

Bravais Lattices

- Only 14 Bravais lattices



http://www.seas.upenn.edu/

Outline

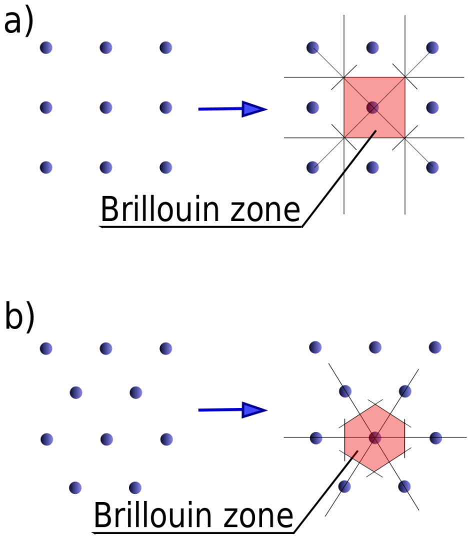
Reciprocal Lattice Vectors

- Solutions to $e^{i\mathbf{K}\cdot\mathbf{r}} = 1$
- Typically form their own Bravais lattice
- Is essentially the Fourier space equivalent of the real space crystal
- Will be related to periodicity of electron plane waves

Brillouin Zones

- Smallest repeating unit in reciprocal space
- Collection of reciprocal vectors that are closest to the 0 vector
- Behavior of electrons in periodic potential characterized by their properties in the first B-Z
- Second, third, etc. Brillouin zones also exist (this periodicity gives rise to bands)

Brillouin Zones



Wikipedia, "Brillouin Zone"

Bloch's Theorem

- $\Psi_{\mathbf{k}}(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(r)$
- Crucially, $u_{\mathbf{k}}(r)$ has (at least some of) the same space group symmetries of the overall reciprocal lattice
- This leads to $\Psi_{\mathbf{k}}(\mathbf{r}+\mathbf{T}) = \Psi_{\mathbf{k}}(\mathbf{r})e^{i\mathbf{k}\cdot\mathbf{T}}$
- For nearly free electrons (NFE), $u_{\mathbf{k}}(r) \approx \frac{1}{\sqrt{\Omega_{\mathbf{r}}}}$
- IMPORTANTLY, $E_{\mathbf{k}+\mathbf{K}} = E_{\mathbf{k}}$

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Space Groups on Reciprocal Vectors

- $\mathbf{T_i} \cdot \mathbf{K_j} = 2\pi N_{ij}$
- $\mathcal{O} T_i \cdot \mathbf{K_j'} = 2\pi N_{ij} \Rightarrow \mathbf{K_j'} = \mathcal{O}^{-1}\mathbf{K_j}$
- The group of all space group transformations which send $\mathbf{k}$ to $\mathbf{k} + \mathbf{K}$ is the **space group of the wave vector**
- For a general Bloch wavefunction, $E_{\mathcal{O}\mathbf{k}} \neq E_{\mathbf{k}}$, BUT if $\mathbf{k}$ is a point of symmetry, all equivalent vectors are degenerate

Representations of Point Groups

- Classes of a point group are equivalent transformations, such as 4-fold rotations or inversions
- Irreducible representations are primarily derived from the Great Orthogonality Theorem
- Irreps of one point group might be decomposable in another related point group
- For a given irrep and Bloch eigenfunction,

$$\mathcal{O}_{R_{\mathbf{k}}} \Psi^{(i)}_{\mathbf{k}\lambda}(\mathbf{r}) = \sum_{\mu} \Psi^{(i)}_{\mathbf{k}\mu}(\mathbf{r}) D^{(i)}(R_{\mathbf{k}})_{\mu\lambda}$$

Character Table for O_h

Repr.	Basis Functions	E	$3C_4^2$	$6C_4$	$6C_2$	$8C_3$	i	$3iC_4^2$	$6iC_4$	$6iC_2$	$8iC_3$
Γ_1	1	1	1	1	1	1	1	1	1	1	1
Γ_2	$\left\{ \begin{array}{l} x^4(y^2-z^2)+ \\ y^4(z^2-x^2)+ \\ z^4(x^2-y^2) \end{array} \right.$	1	1	−1	−1	1	1	1	−1	−1	1
Γ_{12}	$\left\{ \begin{array}{l} x^2-y^2 \\ 2z^2-x^2-y^2 \end{array} \right.$	2	2	0	0	−1	2	2	0	0	−1
Γ_{15}	x, y, z	3	−1	1	−1	0	−3	1	−1	1	0
Γ_{25}	$z(x^2-y^2)$, etc.	3	−1	−1	1	0	−3	1	1	−1	0
Γ_1'	$\left\{ \begin{array}{l} xyz[x^4(y^2-z^2)+ \\ y^4(z^2-x^2)+ \\ z^4(x^2-y^2)] \end{array} \right.$	1	1	1	1	1	−1	−1	−1	−1	−1
Γ_2'	xyz	1	1	−1	−1	1	−1	−1	1	1	−1
Γ_{12}'	$xyz(x^2-y^2)$, etc.	2	2	0	0	−1	−2	−2	0	0	1
Γ_{15}'	$xy(x^2-y^2)$, etc.	3	−1	1	−1	0	3	−1	1	−1	0
Γ_{25}'	xy, yz, zx	3	−1	−1	1	0	3	−1	−1	1	0

Dresselhaus

Compatibility Relations

- Band degeneracies are lifted in moving from a wave vector of high symmetry to one with lower
- The manner in which bands are split is characterized by **compatibility relations**, illustrating irreducible components of now-reducible representations

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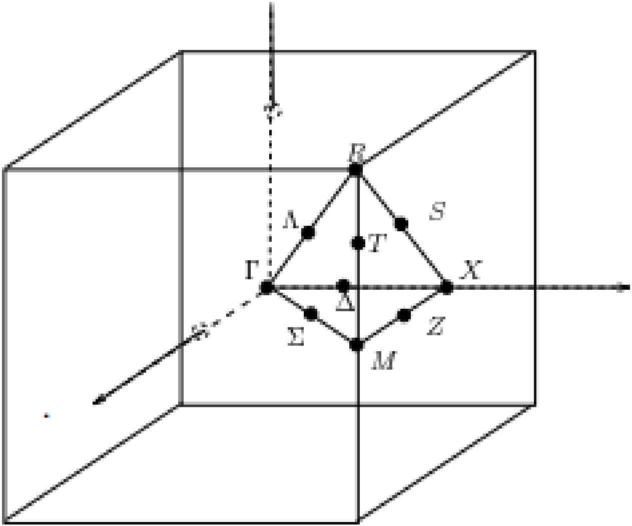
An Example with a Simple Lattice



An Example with a Simple Lattice

the simple cubic lattice.

Compatibility Relations Between Γ and Δ, Λ, Σ.

	Γ_1^+	Γ_2^+	Γ_{12}^+	Γ_{15}^-	Γ_{25}^+	Γ_1^-	Γ_2^-	Γ_{12}^-	Γ_{15}^+	Γ_{25}^-
(100)	Δ_1	Δ_2	$\Delta_1\Delta_2$	$\Delta_1\Delta_5$	$\Delta_{2'}\Delta_5$	$\Delta_{1'}$	$\Delta_{2'}$	$\Delta_{1'}\Delta_{2'}$	$\Delta_{1'}\Delta_5$	$\Delta_2\Delta_5$
(111)	Λ_1	Λ_2	Λ_3	$\Lambda_1\Lambda_3$	$\Lambda_1\Lambda_3$	Λ_2	Λ_1	Λ_3	$\Lambda_2\Lambda_3$	$\Lambda_2\Lambda_3$
(110)	Σ_1	Σ_4	$\Sigma_1\Sigma_4$	$\Sigma_1\Sigma_3\Sigma_4$	$\Sigma_1\Sigma_2\Sigma_3$	Σ_2	Σ_3	$\Sigma_2\Sigma_3$	$\Sigma_2\Sigma_3\Sigma_4$	$\Sigma_1\Sigma_2\Sigma_4$

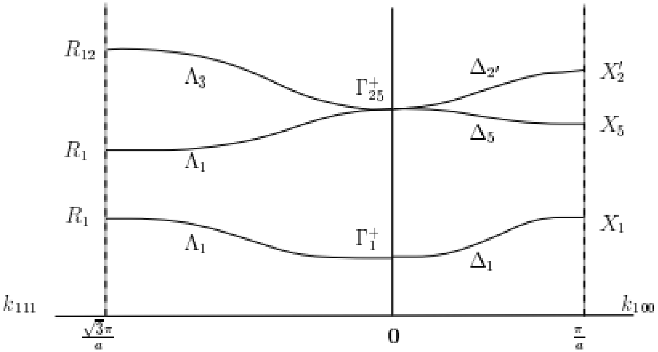
Compatibility Relations Between X and Δ, Z, S

X_1	X_2	X_3	X_4	X_5	$X_{1'}$	$X_{2'}$	$X_{3'}$	$X_{4'}$	$X_{5'}$
Δ_1	Δ_2	$\Delta_{2'}$	$\Delta_{1'}$	Δ_5	$\Delta_{1'}$	$\Delta_{2'}$	Δ_2	Δ_1	Δ_5
Z_1	Z_1	Z_4	Z_4	Z_3Z_2	Z_2	Z_2	Z_3	Z_3	Z_1Z_4
S_1	S_4	S_1	S_4	S_2S_3	S_2	S_3	S_2	S_3	S_1S_4

Compatibility Relations Between M and Σ, Z, T

M_1	M_2	M_3	M_4	$M_{1'}$	$M_{2'}$	$M_{3'}$	$M_{4'}$	M_5	$M_{5'}$
Σ_1	Σ_4	Σ_1	Σ_4	Σ_2	Σ_3	Σ_2	Σ_3	$\Sigma_2\Sigma_3$	$\Sigma_1\Sigma_4$
Z_1	Z_1	Z_3	Z_3	Z_2	Z_2	Z_4	Z_4	Z_2Z_4	Z_1Z_3
T_1	T_2	$T_{2'}$	$T_{1'}$	$T_{1'}$	$T_{2'}$	T_2	T_1	T_5	T_5

An Example with a Simple Lattice



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Perturbation Theory

$$\left[\frac{p^2}{2m} + V(\mathbf{r}) + \frac{\hbar\mathbf{k}\cdot\mathbf{p}}{m} + \frac{\hbar^2 k^2}{2m}\right] u_{n,\mathbf{k}}(\mathbf{r}) = E_n(\mathbf{k}) u_{n,\mathbf{k}}(\mathbf{r})$$

- Energy is assumed known at some $\mathbf{k_0}$, and the wave vector has some symmetry Γ_i
- Then Schrödinger becomes $H_{\mathbf{k_0}} u^{(\Gamma_i)}_{n,\mathbf{k_0}}(\mathbf{r}) = \epsilon_n(\mathbf{k_0}) u^{(\Gamma_i)}_{n,\mathbf{k_0}}(\mathbf{r})$
- For a small perturbation, $\left(H_{\mathbf{k_0}} + \frac{\hbar\kappa\cdot\mathbf{p}}{m}\right) u^{(\Gamma_i)}_{n,\mathbf{k_0}+\kappa}(\mathbf{r}) = \epsilon_n(\mathbf{k_0}+\kappa) u^{(\Gamma_i)}_{n,\mathbf{k_0}+\kappa}(\mathbf{r})$

Selection Rules

- Suppose we want to calculate the matrix element $\left\langle \Phi^{(i)} | H' | \Phi^{(j)} \right\rangle$
- Under space group operations which respect the Hamiltonian, this matrix element must either be constant or trivially zero, depending on whether the wavefunctions provided transform like equivalent representations
- More concretely, if the matrix element transforms as $\Gamma_i \otimes \Gamma_n \otimes \Gamma_j$, then either $(\Gamma_n \otimes \Gamma_j)$ is orthogonal to Γ_i, or the direct product is a constant.

Outline

Introduction to Crystals
- Bravais Lattices
- Brillouin Zones

Groups and Basic Band Theory
- Space Group Representations
- Simple Cubic Example

Perturbation on Bands
- $\mathbf{k} \cdot \mathbf{p}$ Perturbation Theory
- Selection Rules in Action

Selection Rules in Action

- We can see these selection rules in action by returning to our band perturbation theory
- Let us look at the Γ_1^+ band from the $\mathbf{0}$ vector in a simple cubic lattice

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$$\epsilon_n^{(\Gamma_1)}(\kappa) = E_n(\mathbf{0}) + \left\langle u_{n,\mathbf{0}}^{\Gamma_1} | H' | u_{n,\mathbf{0}}^{\Gamma_1} \right\rangle$$

$$+ \sum_{n' \neq n} \frac{\left\langle u_{n,\mathbf{0}}^{\Gamma_1} | H' | u_{n',\mathbf{0}}^{\Gamma_i} \right\rangle \left\langle u_{n',\mathbf{0}}^{\Gamma_i} | H' | u_{n,\mathbf{0}}^{\Gamma_1} \right\rangle}{E_n^{\Gamma_1}(\mathbf{0}) - E_{n'}^{\Gamma_i}(\mathbf{0})}$$

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- $H' = \frac{\hbar\kappa\cdot\mathbf{p}}{m}$ is a vector, and so transforms like the Γ_{15}^{-} representation of O_h
- This means that the linear term vanishes, as $\Gamma_{15}^{-} \otimes \Gamma_1^{+} = \Gamma_{15}^{-} \neq \Gamma_1^{+}$
- Looking at the second order terms, we realize the expression simplifies to $\frac{\left\langle u_{n,\mathbf{0}}^{\Gamma_1^+} | H' | u_{n',\mathbf{0}}^{\Gamma_{15}^-} \right\rangle \left\langle u_{n',\mathbf{0}}^{\Gamma_{15}^-} | H' | u_{n,\mathbf{0}}^{\Gamma_1^+} \right\rangle}{E_n^{\Gamma_1^+}(\mathbf{0}) - E_{n'}^{\Gamma_{15}^-}(\mathbf{0})}$

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- After some simplification with appropriate basis functions, we get

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$$E_n^{\Gamma_1^+}(\kappa) = E_n^{\Gamma_1^+}(\mathbf{0}) + \frac{\hbar^2\kappa^2}{2m}$$

$$+\frac{\hbar^2\kappa^2}{m^2}\sum_{n\neq n'}\frac{\left\langle S|\mathbf{p}|P\right\rangle^2}{E_n^{\Gamma_1^+}(\mathbf{0}) - E_{n'}^{\Gamma_{15}^-}(\mathbf{0}}$$

Summary

- A working knowledge of the group theory of point and space groups is incredibly useful in the field of theoretical solid state physics
- One particular application is in the analysis of bands around points of high symmetry in the reciprocal lattice
- We looked at how these tools can be used to predict band energies close to symmetric points in a particular perturbation model

Bibliography I

D. Bishop
Group Theory and Chemistry

M. S. Dresselhaus.
Applications of Group Theory to the Physics of Solids.

V. Heine
Group Theory in Quantum Mechanics

M. P. Marder
Condensed Matter Physics