Band representations

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Part 1: Building band representations

Sec II and Appendix B
Space groups describe symmetry of 3D crystals

Ex: P6mm, (#183)
C₆z, mₓ, lattice translations

Real space

Brillouin zone
Within one space group, many ways to arrange atoms

1 atom/unit cell (triangular)

2 atoms/unit cell (honeycomb)

3 atoms/unit cell (kagome)

All atoms are related by symmetry
Within one arrangement, many choices of orbitals

- s (or $p_z$) orbitals
- 2 atoms/unit cell
- $p_x$ and $p_y$ orbitals
Each arrangement/orbital determines symmetry representations in Brillouin zone.

**s (or p_z) orbitals**

**p_x and p_y orbitals**

Real space vs momentum space
Input real space symmetry

1. space group
2. atom positions
3. orbitals

Band representation: atomic limit and its symmetry

Brillouin zone symmetry

\( \Gamma_1 \quad \Gamma_4 \quad K_3 \quad M_1 \quad M_4 \)
How to build a band representation? First, define basis

Consider one lattice site:

Site-symmetry group, $G_q$, leaves $q$ invariant $C_3, m_y$

Orbitals at $q$ transform under a rep, $\rho$, of $G_q$

Elements of space group $g \not\in G_q$ move sites in an orbit “Wyckoff position” $C_6$
Mathematical tool: coset decomposition

• Given a group $G$, and a subgroup, $H$, then $G$ can always be partitioned as:

$$G = \bigcup_{\alpha} g_{\alpha}H = g_1H + g_2H + \cdots + g_nH$$

**Example for finite groups:**

$$G = C_{6v}, \ H = C_{2v} \quad G = EC_{2v} \cup C_3C_{2v} \cup C_3^2C_{2v}$$

**Example for infinite groups:**

$$G = \mathbb{Z}, \ H = 4\mathbb{Z} \quad G = (4\mathbb{Z} + 0) \cup (4\mathbb{Z} + 1) \cup (4\mathbb{Z} + 2) \cup (4\mathbb{Z} + 3)$$

**Two trivial cases:**

$$H = G \Rightarrow G = EH \quad H = E \Rightarrow G = \bigcup_{g \in G} gH$$
How to build a band representation? First, define basis

Band rep defined by:
- space group, \( G \)
- atomic position, \( q \)
- orbital, \( \rho \)

\( \rho \) is a representation of the site-symmetry group:
\[
G_q = \{ g | gq = q \} \subset G
\]

Coset decomposition:
\[
G = \bigcup_{\alpha} g_\alpha (G_q \rtimes \mathbb{Z}^3)
\]

Coset representatives move between sites:
\[
q_\alpha \equiv g_\alpha q
\]

Site-symmetry group elements rotate between orbitals
\[
q_1 = C_6 q
\]

Tight-binding basis:
\[
| \phi_{R, \alpha, i} \rangle \equiv T_R g_\alpha | \phi_{0, 1, 1} \rangle
\]

unit cell \hspace{1cm} atom \hspace{1cm} orbital
How does symmetry act in real space?

By virtue of being in site-symmetry group:

\[
\langle \phi_{0,1,j} | g | \phi_{0,1,i} \rangle = \rho(g)_{ji}, \quad g \in G_q
\]

What about elements not in the site-symmetry group? \( h=\{P|v\} \)

\[
h|\phi_{R,\alpha i} \rangle = \{P|v\}\{E|R\}g_\alpha |\phi_{0,1,i} \rangle
\]

\[
= \{E|PR\}\{P|v\}g_\alpha |\phi_{0,1,i} \rangle
\]

use coset decomposition!

\[
h g_\alpha = \{E|t\} g_\beta g
\]

= \{E|PR + t\}g_\beta |\phi_{0,1,j} \rangle [\rho(g)]_{ji}

= |\phi_{PR+t,\beta j} \rangle [\rho(g)]_{ji}

Orbital part of U is exactly \( \rho \); site index from coset decomposition, i.e., \( \alpha \rightarrow \beta \)
Result: \[ h|\phi_{R,\alpha_i}\rangle = |\phi_{PR+t,\beta_j}\rangle [\rho(g)]_{ji} \]

where \(t, g\) and \(\beta\) are defined by the coset decomposition:

\[ hg_\alpha = \{E|t\}\ g_\beta g \]

This is the general formula for finding the matrix \(U\) from yesterday

Recall definition of \(U\):

\[ h|\phi_{R,\alpha_i}\rangle = [U_h]_{\beta_j,\alpha_i} |\phi_{R',\beta_j}\rangle \]
How to find little co-group irreps

\[ h|\phi_{R,\alpha}i \rangle = [U_h]_{\beta j, \alpha i} |\phi_{R', \beta}i \rangle \]

Fourier transform:

\[ h|\chi^{Pk}_{\alpha i} \rangle = |\chi^{Pk}_{\beta j} \rangle [U_h]_{\beta j, \alpha i} e^{-i(Pk) \cdot v} \]

If g is in the little co-group at k:

\[ h|\chi^{k}_{\alpha i} \rangle = |\chi^{k}_{\beta j} \rangle [V(G)^{-1}U_h]_{\beta j, \alpha i} e^{-i(Pk) \cdot v}, \ Pk = k + G \]

Character of \( h=\{P,v\} \) is given by trace:

\[ \text{Tr} \left[ V(G)^{-1}U_h \right] e^{-i(Pk) \cdot v}, \ Pk = k + G \]
Each atomic limit defines a band representation

A band representation is a representation of the space group
It is induced by a representation of a site-symmetry group

Each symmetry operation represented by \( N \times N \) matrix

<table>
<thead>
<tr>
<th></th>
<th>( q )</th>
<th>( q_2 )</th>
<th>( q_3 )</th>
<th>( q_4 )</th>
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</tr>
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<tr>
<td>( q )</td>
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</table>

Diagonal block if \( g \in G_q \), i.e., \( gq = q \)

Off-diagonal block if \( g \) interchanges sites

The symmetry irreps of a band representation in the Brillouin zone are completely determined.


Diagonal blocks are rep. of site-symmetry group, $G_q$

Diagonal blocks form rep. of “little group of $k_i$”
Example: band representation of 1D lattice with inversion symmetry

\[ G_q = \{ E, I \} \quad G = E G_q \times T \Rightarrow g_1 = E \]

Coset decomposition for inversion:

\[ I g_1 = \{ E|0 \} g_1 I \]

\[ I |\phi_R\rangle = |\phi_{-R}\rangle \rho(I) \]

Since there are no other sites, this is exactly \( \mathbf{U} \)

Conclusion: for s orbitals, \( \mathbf{U} = (1) \), and for p orbitals, \( \mathbf{U} = (-1) \)

As we asserted yesterday, for s and p orbitals, \( \mathbf{U}_I = \begin{pmatrix} +1 \\ -1 \end{pmatrix} \)
To find little group irreps, plug into the character formula:

Character of \( h = \{ P, v \} \) is given by trace:

\[
\text{Tr} \left[ V(G)^{-1} U_h \right] e^{-i(Pk) \cdot v}, \quad Pk = k + G
\]

**Simplifications:**

\[ V(G) = I \] because atoms at \( r = 0 \)

\[ v = 0 \] because we are only considering inversion

**Character table**

<table>
<thead>
<tr>
<th>( C_i(-1) )</th>
<th>( \Gamma_1^+ )</th>
<th>1</th>
<th>1</th>
</tr>
</thead>
<tbody>
<tr>
<td>( A_g )</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>( A_u )</td>
<td>1</td>
<td>-1</td>
<td></td>
</tr>
</tbody>
</table>

At both \( k = 0 \) and \( k = \pi \), the character is \( \text{Tr}[U_i] = \text{Tr}[\rho(I)] \)

For s orbital: \( \text{Tr}[U_i] = +1 \Rightarrow A_g \)

For p orbitals: \( \text{Tr}[U_i] = -1 \Rightarrow A_u \)
Example: band representation of 1D lattice with inversion, atoms at general position

\[ G_q = \{ E \} \]

\[ G = (E G_q \cup I G_q) \ltimes T \]

\[ g_1 = E, g_2 = I \]

Coset decomposition for inversion:

\[ I g_1 = \{ E \vert 0 \} g_2 E \]

\[ I g_2 = \{ E \vert 0 \} g_1 E \]

Conclusion: as we asserted yesterday,

\[ U_I = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \]
To find little group irreps, plug into the character formula:

Character of \( h=\{P,v\} \) is given by trace:

\[
\text{Tr} \left[ V(G)^{-1} U_h \right] e^{-i(Pk) \cdot v}, \quad Pk = k + G
\]

Simplification:

\[
V(G) = \begin{pmatrix} e^{iG \cdot x_0} & 0 \\ 0 & e^{-iG \cdot x_0} \end{pmatrix}
\]

\[
\text{Tr} \left[ V(G)^{-1} U_h \right] = \text{Tr} \left( \begin{pmatrix} 0 & e^{iG \cdot x_0} \\ e^{-iG \cdot x_0} & 0 \end{pmatrix} \right) = 0
\]

Character table

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<td>( \Gamma_1^- )</td>
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</tr>
</tbody>
</table>

At both \( k=0 \) and \( k=\pi \), the character is 0

2d rep with zero inversion character: \( A_g \oplus A_u \)
Part 2: Elementary band representations

Refs: “Topological quantum chemistry,”
Bradlyn, Elcoro, Cano, Vergniory, Wang, Felser, Aroyo, Bernevig

“Building blocks of topological quantum chemistry,”
Cano, Bradlyn, Wang, Elcoro, Vergniory, Felser, Aroyo, Bernevig
Secs II and III
Band representations can describe multiple orbitals in different positions

Infinitely many band representations!
Elementary band reps are the building blocks
Elementary band representations do not decompose into sum of band representations

1. Elementary band reps are induced from irreducible representations of $G_q$

\[
(r_1 \oplus r_2)^\uparrow G = (r_1^\uparrow G) \oplus (r_2^\uparrow G)
\]

2. All EBRs can be induced from representations of maximal site-symmetry groups

\[
(r^\uparrow H)^\uparrow G = r^\uparrow G \\
K \subset H \subset G
\]

$\Rightarrow$ Finitely many EBRs
How many EBRs are there?

- This is the process by which we have enumerated all the EBRs that appear on the BCS (modulo exceptions).

- Large but finite number, estimate:

\[(230 \text{ space groups}) \times (3 \text{ max Wyckoff pos.}) \times (3 \text{ irreps}) = 2070\]

<table>
<thead>
<tr>
<th>Actual:</th>
<th>no TR</th>
<th>TR</th>
</tr>
</thead>
<tbody>
<tr>
<td>Single-valued irreps (spinless)</td>
<td>3383</td>
<td>3141</td>
</tr>
<tr>
<td>Double-valued irreps (spinful)</td>
<td>2263</td>
<td>1616</td>
</tr>
</tbody>
</table>

⇒ 10,403 total EBRs
Decomposition into band representations is not unique

Consider site $\mathbf{q}$, site-symmetry group $G_q$

Consider site $\mathbf{q}'$, site-symmetry group $G_{q'}$

Let $G_0 = G_q \cap G_{q'}$

If there is a site, $\mathbf{q}_0$, with site-symmetry group $G_0$, then a rep $\sigma$ of $G_0$ induces the same band rep as $\sigma \uparrow G_q$ and as $\sigma \uparrow G_{q'}$

$$\sigma \uparrow G = (\sigma \uparrow G_q) \uparrow G = (\sigma \uparrow G_{q'}) \uparrow G$$
Summary

• Real space symmetry determines a band representation.

• The little co-group irreps of a band representation are completely determined.

• Elementary band representations cannot be written as a sum of other band representations.
Exercises

Compute the band representation in 1d with inversion, atom at q=1/2.

a) What is the site-symmetry group? Hint: it does not contain inversion because inversion takes q = 1/2 → -1/2.

b) What are the two irreps of the site-symmetry group?

c) What are the cosets of the space group with respect to the site-symmetry group? How many coset representatives are there? (Does this explain why q=1/2 is called the 1b position?)

d) What is the coset decomposition of hg_α, where h = inversion and g_α is a coset representative?

e) Given an irrep of the site-symmetry group, write the matrix U in terms of the irrep.

f) Apply the character formula to find the character of inversion at k=0 and k=π, for each of the irreps of the site-symmetry group. (Hint: \( v = 0 \) because inversion is a point group operation. But \( G \) is different at \( k=0 \) and \( k=\pi \). What irrep appears at \( k=0? \ k=\pi? \)

 g) Now consider the band rep induced from a sum of both irreps of the site-symmetry group. The little co-group irreps are the sum of those from each band rep individually. How does this sum compare to what we found in the lecture for q=0? How does it compare to q=x_0, 0< x_0 < 1/2.

h) Explain why the three band representations are the same.
Exercises, cont.

Band representation for \(\text{p4mm}\).

a) For \(q=(0,0)\), what is the site-symmetry group? What is \(\rho(g)\) for \(s\) orbitals? What about \(p_x\) and \(p_y\) orbitals? Why didn’t I ask for \(p_z\) orbitals?

b) For \(q’=(1/2,0)\), what is the site-symmetry group? What is \(\rho(g)\) for \(s\) orbitals? What about \(p_x\) and \(p_y\) orbitals?

c) Use the coset decomposition to compute the matrix representations and little co-group irreps in each case.

Coset decomposition.

a) Prove that in the coset decomposition: 
\[
hg_\alpha = \{E|t\} g_\beta g, \ t = hq_\alpha - q_\beta
\]

Hint: act with both sides on the site \(q\). Also recall \(q_\alpha = g_\alpha q\).

b) Why must \(t\) be a lattice vector to be a solution to the equation?

c) Recalling, \(PR + t = R’\), prove yesterday’s equation for the same symmetry operation:
\[
P(R + q_\alpha) + v = R’ + q_\beta
\]