Band representations

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Part 1: Building band representations

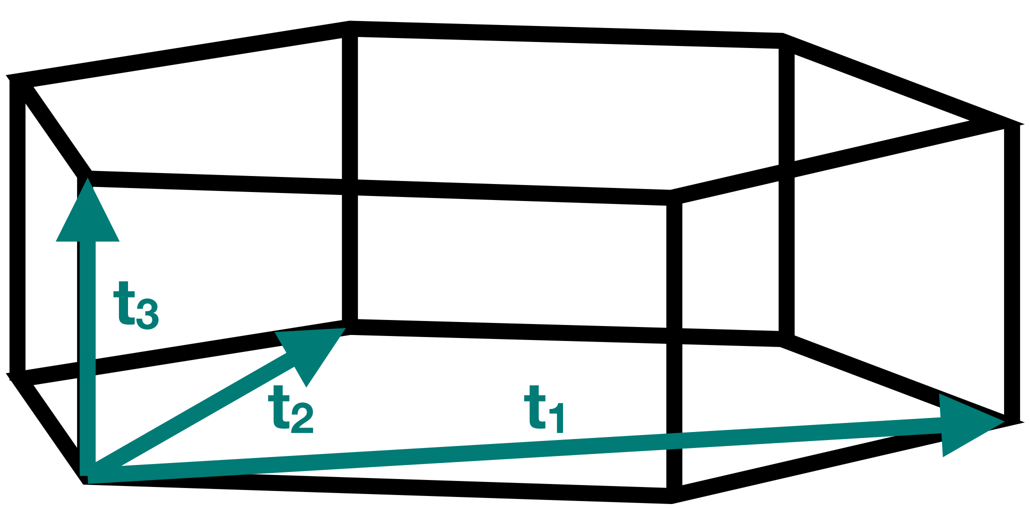
Ref: "Building blocks of topological quantum chemistry,"
Cano, Bradlyn, Wang, Elcoro, Vergniory, Felser, Aroyo, Bernevig
ArXiv: 1709.01935, PRB 97, 035139 (2018)
Sec II and Appendix B

Space groups describe symmetry of 3D crystals

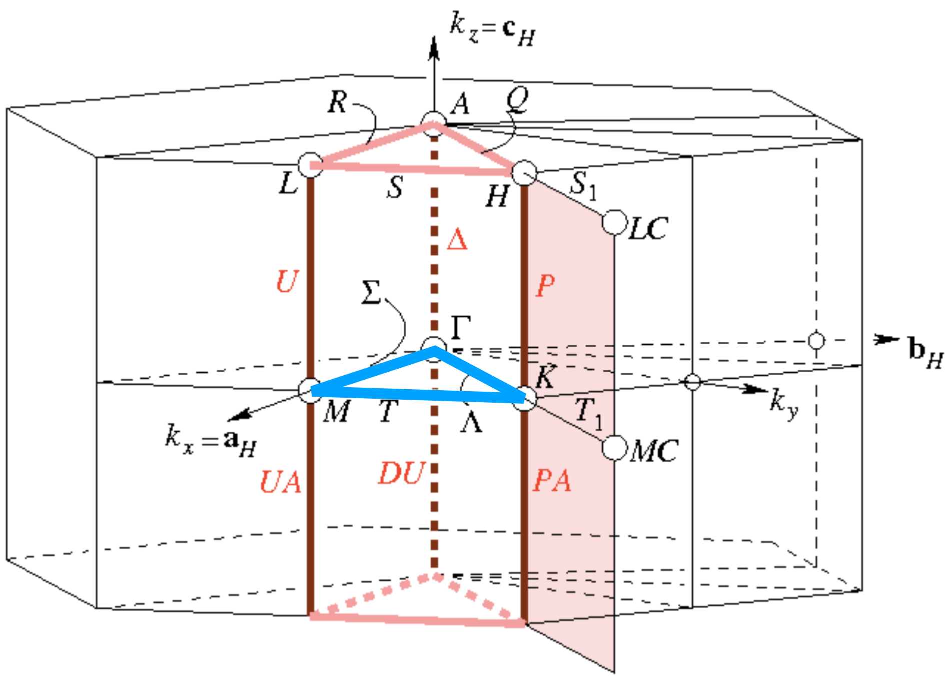
Ex: P6mm, (#183)

C_{6z}, m_x, lattice translations

Real space



Brillouin zone



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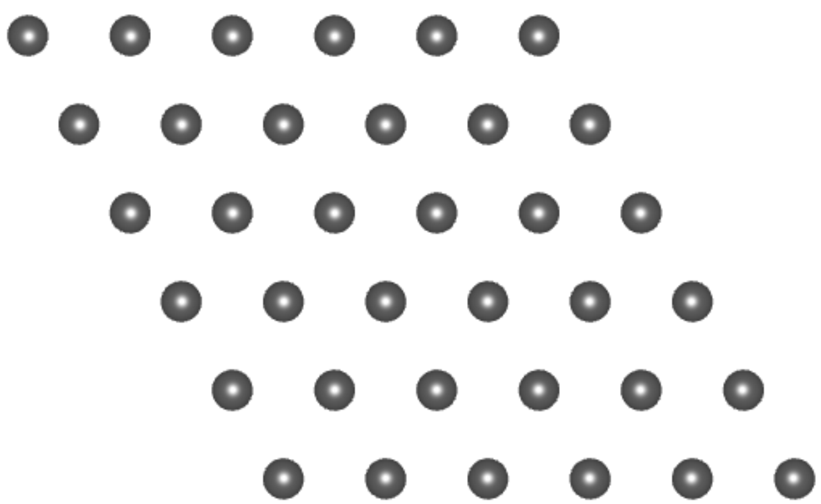
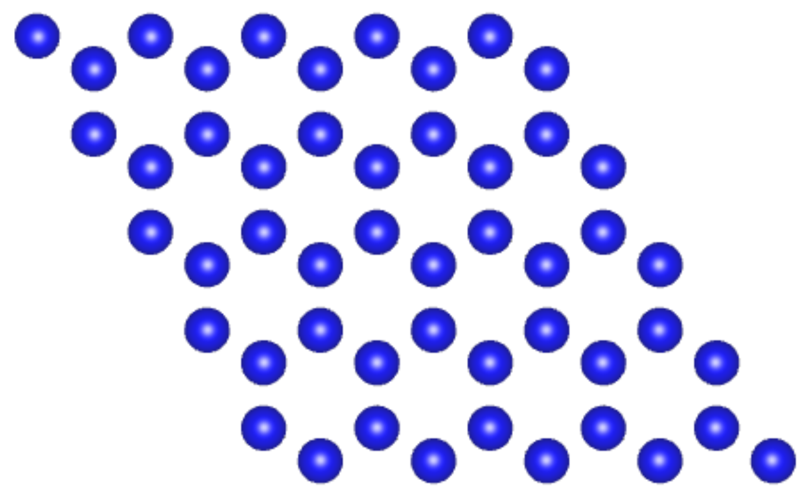
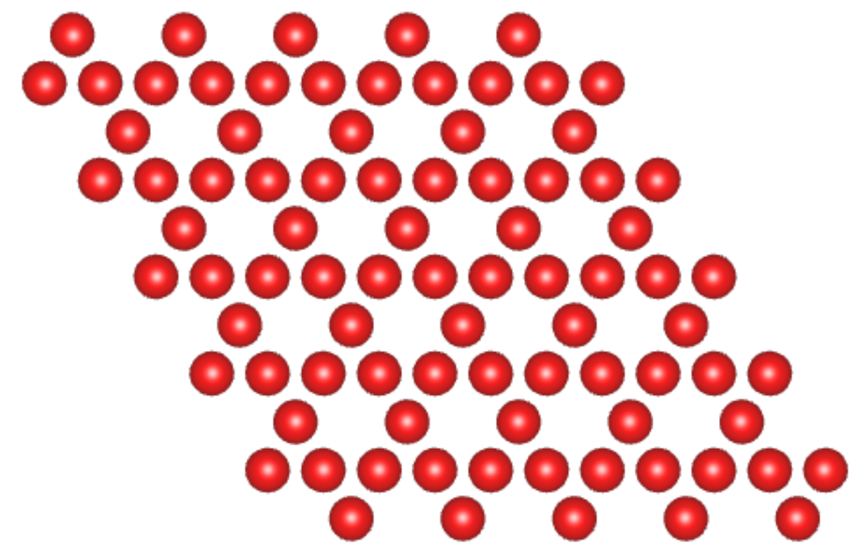
Within one space group, many ways to arrange atoms



1 atom/unit cell
(triangular)



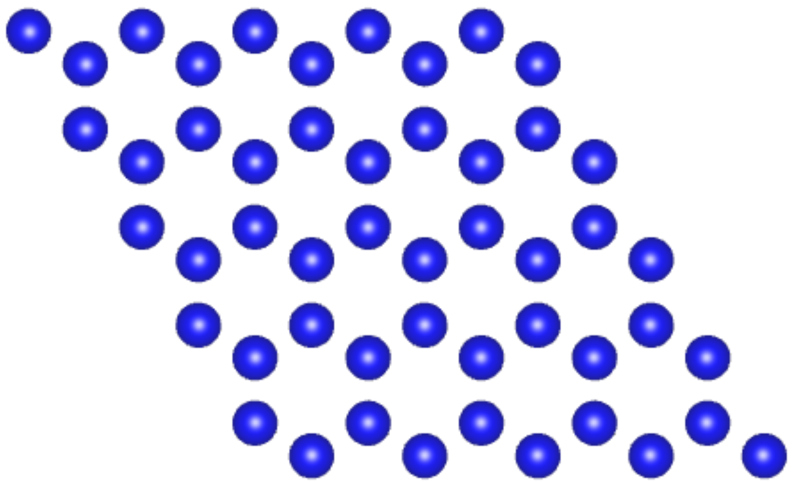
2 atoms/unit cell
(honeycomb)



3 atoms/unit cell
(kagome)

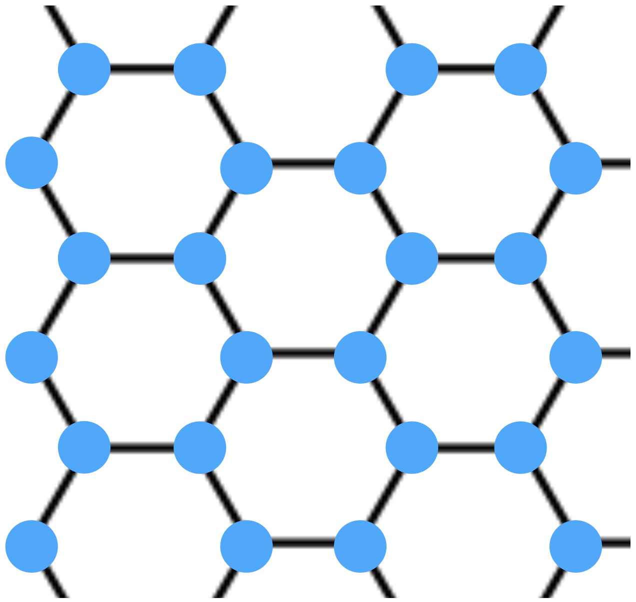
All atoms are related by symmetry

Within one arrangement, many choices of orbitals

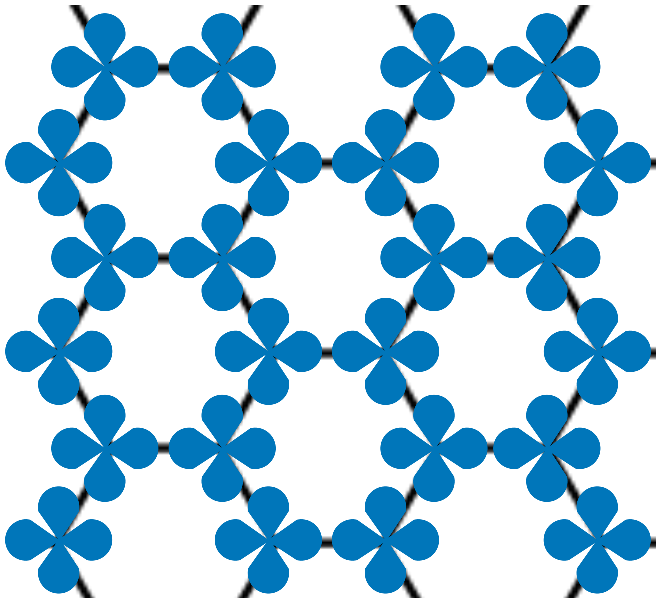


2 atoms/unit cell

s (or p_z) orbitals

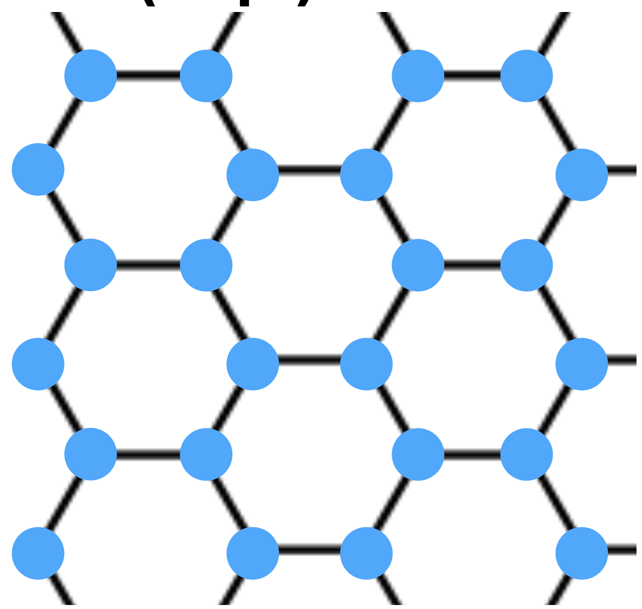


p_x and p_y orbitals

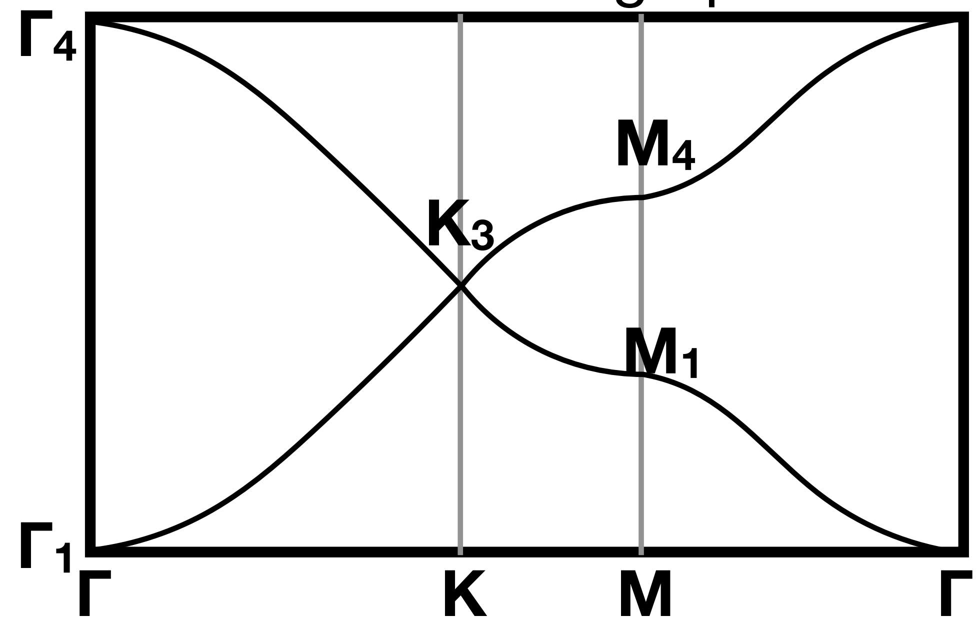


Each arrangement/orbital determines symmetry representations in Brillouin zone

s (or p_z) orbitals

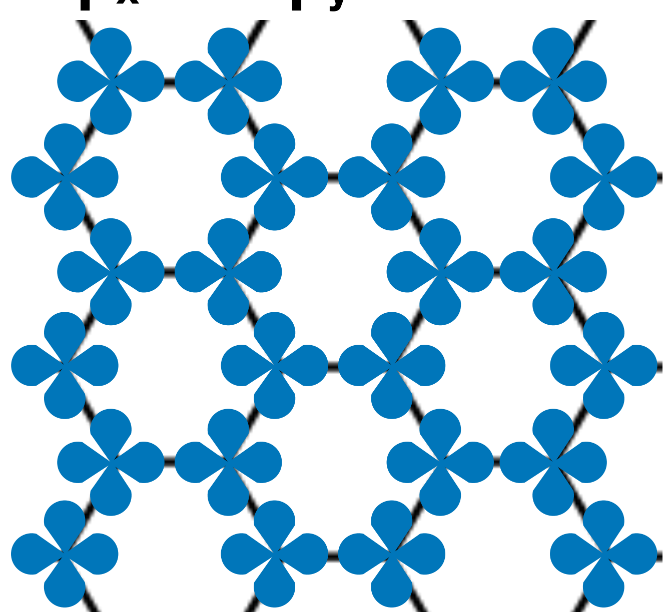


Band structure graphene

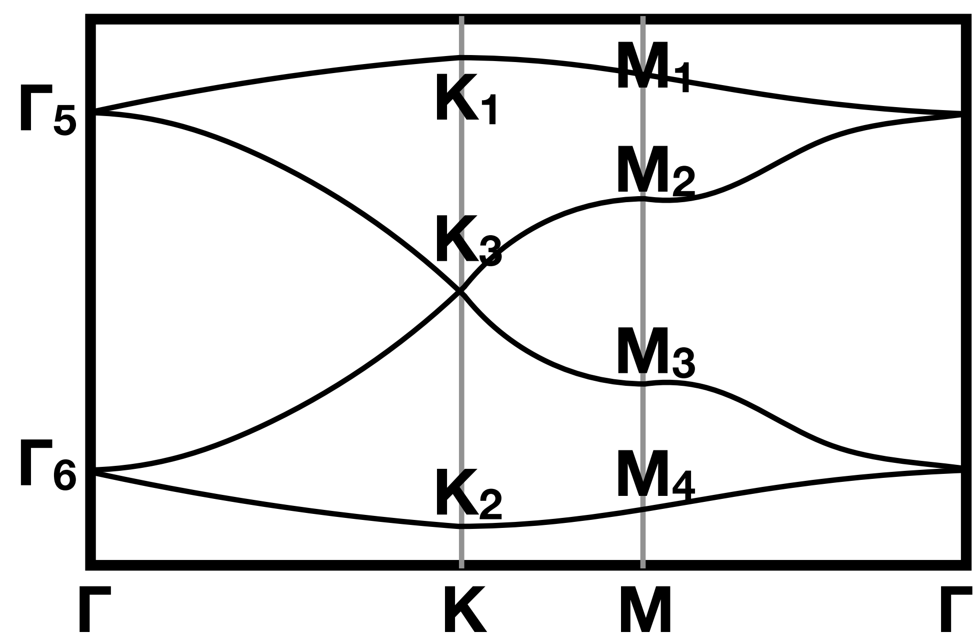


Real space vs momentum space

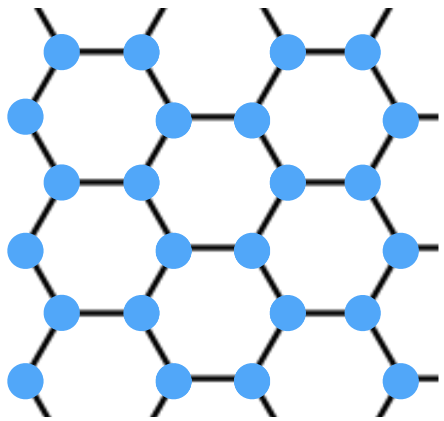
p_x and p_y orbitals



Band structure bismuthene



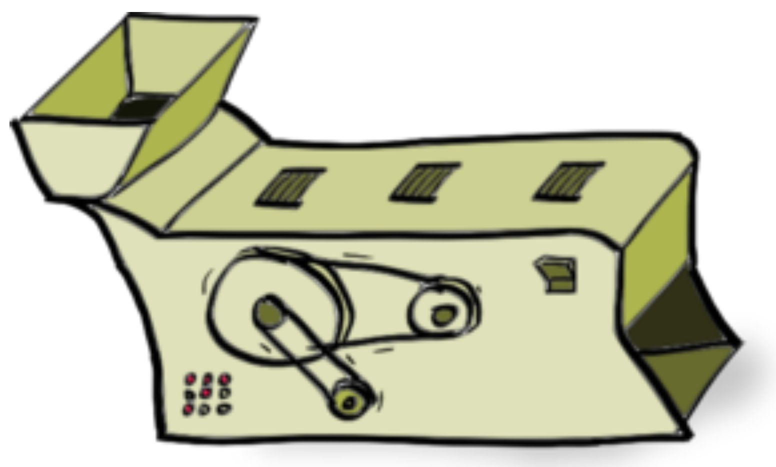
Input real space symmetry



1. space group
2. atom positions
3. orbitals

Band representation: atomic limit and its symmetry

Zak PRL 1980, PRB 1981, 1982

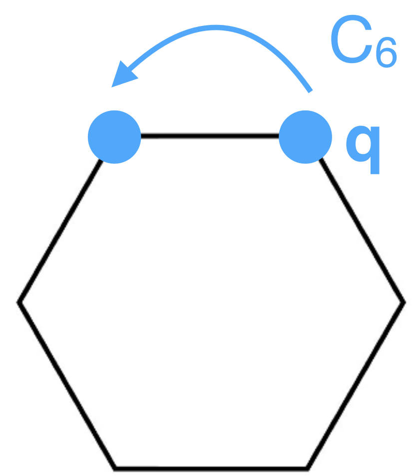


Brillouin zone symmetry

Γ_1 Γ_4 K_3 M_1 M_4

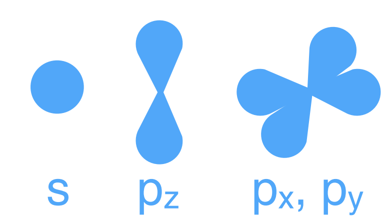
How to build a band representation? First, define basis

Consider one lattice site:



Site-symmetry group, $G_{\mathbf{q}}$, leaves **q** invariant C_3, m_y

Orbitals at **q** transform under a rep, ρ, of $G_{\mathbf{q}}$



Elements of space group $g \notin G_{\mathbf{q}}$ 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:

$$G = \bigcup_{\alpha} g_\alpha H = g_1 H + g_2 H + \cdots + g_n H$$

coset representatives

Example for finite groups:

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

Example for infinite groups:

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

Two trivial cases:

$$H = G \Rightarrow G = EH \qquad H = E \Rightarrow G = \bigcup_{g \in G} gH$$

How to build a band representation? First, define basis

Band rep defined by:
space group, **G**
atomic position, **q**
orbital, **ρ**

ρ is a representation of the site-symmetry group:

$$G_{\mathbf{q}} = \{g | g\mathbf{q} = \mathbf{q}\} \subset G$$

Coset decomposition:

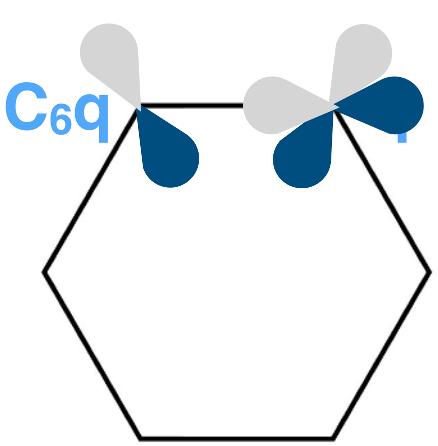
$$G = \bigcup_{\alpha} \overbrace{g_\alpha}^{\text{finite}} (G_{\mathbf{q}} \ltimes \mathbb{Z}^3)$$

coset representatives

Coset representatives move between sites: $\mathbf{q}_\alpha \equiv g_\alpha \mathbf{q}$

Site-symmetry group elements rotate between orbitals

$\mathbf{q}_1 = C_6\mathbf{q}$



Tight-binding basis:

$$|\phi_{\mathbf{R},\alpha,i}\rangle \equiv T_{\mathbf{R}} g_\alpha |\phi_{\mathbf{0},1,1}\rangle$$

unit cell atom orbital

How does symmetry act in real space?

By virtue of being in site-symmetry group:

$$\langle \phi_{\mathbf{0},1,j} | g | \phi_{\mathbf{0},1,i} \rangle = \rho(g)_{ji}, \;\; g \in G_{\mathbf{q}}$$

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

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

$$= \{E|P\mathbf{R}\}\{P|\mathbf{v}\}g_\alpha|\phi_{\mathbf{0},1,i}\rangle$$

use coset decomposition!

$$hg_\alpha = \{E|\underset{\text{lattice vec}}{\mathbf{t}}\}\underset{\text{coset rep.}}{g_\beta}\underset{\text{element of } G_{\mathbf{q}}}{g}$$

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

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

Orbital part of U is exactly ρ; site index from coset decomposition, i.e., α→β

Result: $$h|\phi_{\mathbf{R},\alpha i}\rangle = |\phi_{P\mathbf{R}+\mathbf{t},\beta j}\rangle\,[\rho(g)]_{ji}$$

where **t**, *g* and β are defined by the coset decomposition: $$hg_\alpha = \{E|\mathbf{t}\}g_\beta g$$

<u>**This is the general formula for finding the matrix U from yesterday**</u>

Recall definition of U: $$h|\phi_{\mathbf{R},\alpha i}\rangle = [U_h]_{\beta j,\alpha i}\,|\phi_{\mathbf{R}',\beta j}\rangle$$

How to find little co-group irreps

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

Fourier transform:

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

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

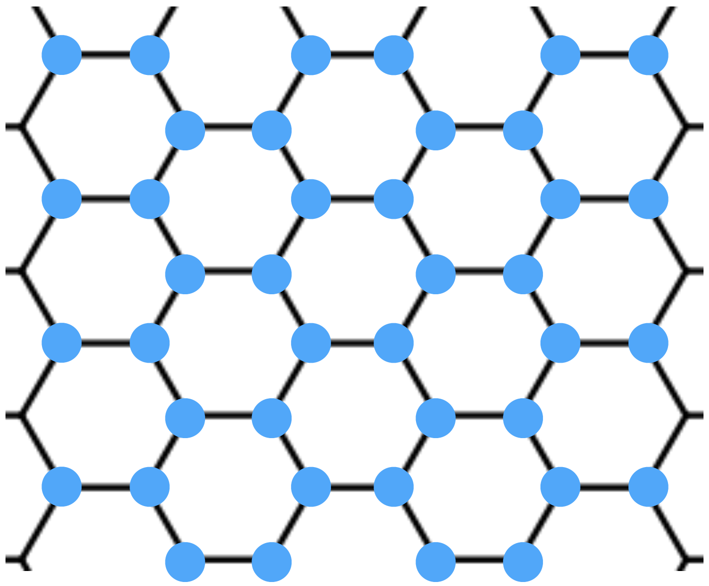
$$h|\chi^{\mathbf{k}}_{\alpha i}\rangle = |\chi^{\mathbf{k}}_{\beta j}\rangle[V(\mathbf{G})^{-1}U_h]_{\beta j,\alpha i}e^{-i(P\mathbf{k})\cdot\mathbf{v}},\ P\mathbf{k} = \mathbf{k}+\mathbf{G}$$

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

$$\mathrm{Tr}\left[V(\mathbf{G})^{-1}U_h\right]e^{-i(P\mathbf{k})\cdot\mathbf{v}},\ P\mathbf{k} = \mathbf{k}+\mathbf{G}$$

Each atomic limit defines a band representation

Zak PRL 1980, PRB 1981, 1982



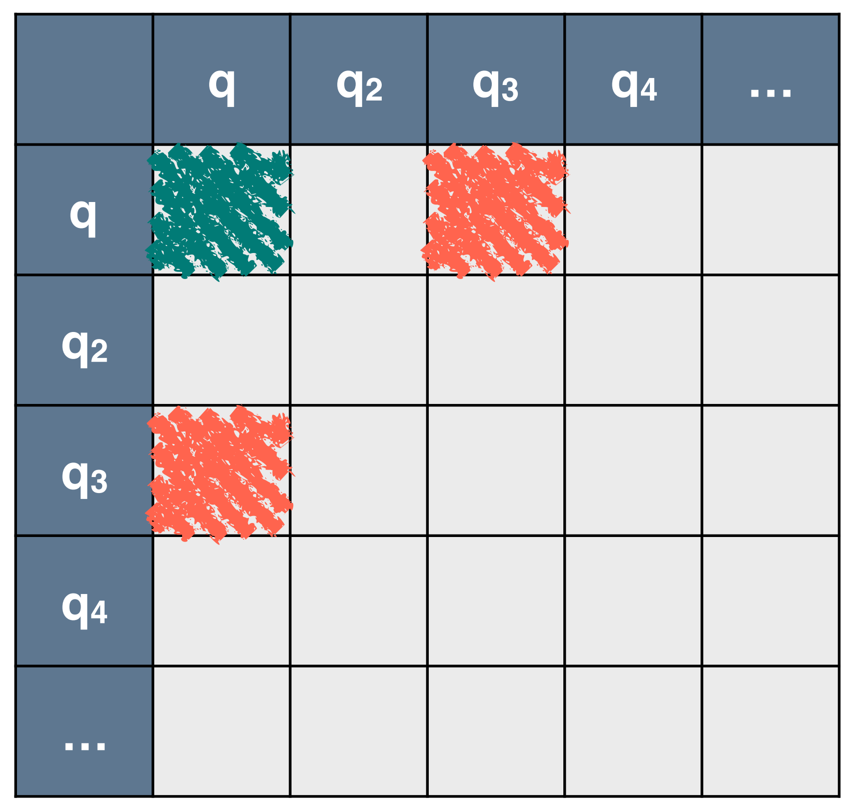
A band representation is a representation of the space group

It is induced by a representation of a site-symmetry group

Each symmetry operation represented by N x N matrix

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

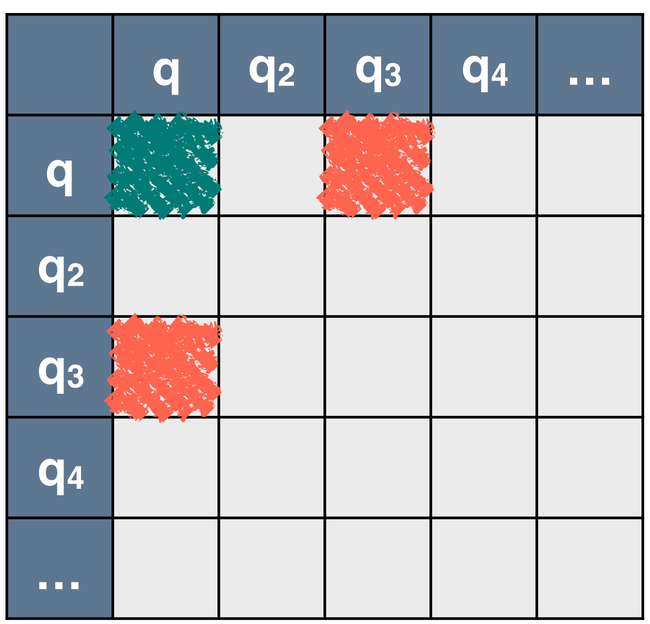
Off-diagonal block if g interchanges sites



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

Zak PRL 1980, PRB 1981, 1982

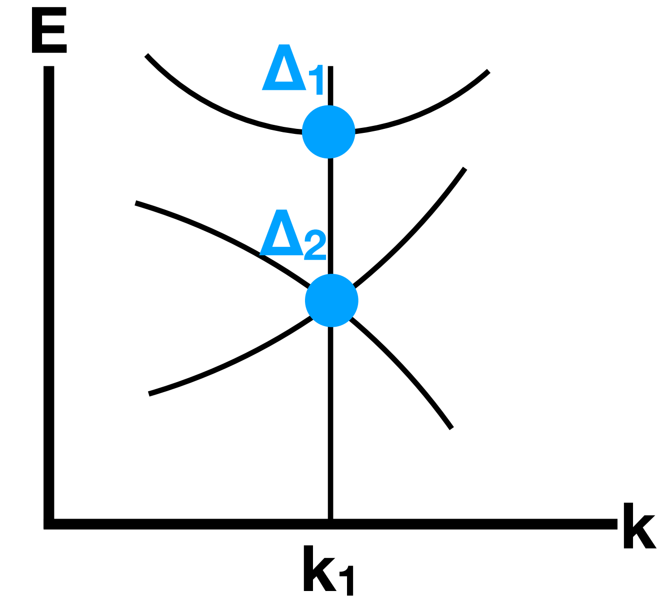
Real space rep.



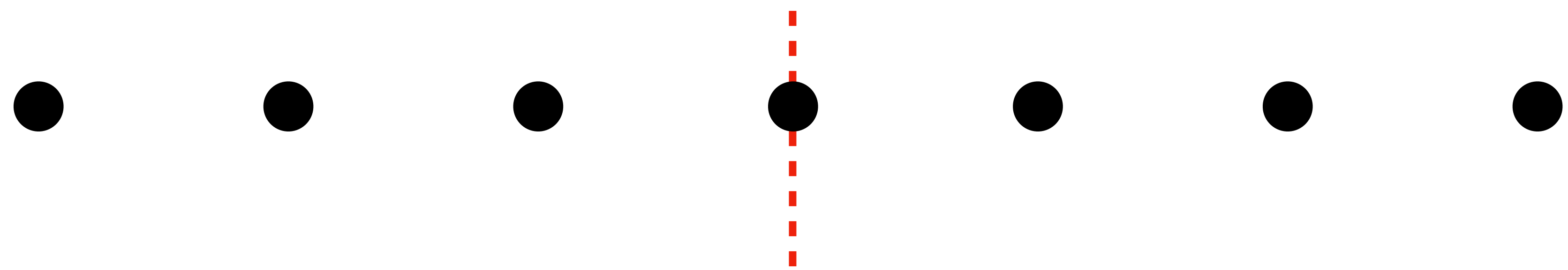
Diagonal blocks are rep. of site-symmetry group, G_q

Fourier transformed rep.

Diagonal blocks form rep. of "little group of k_i"



Example: band representation of 1D lattice with inversion symmetry



$$G_{\mathbf{q}} = \{E, I\} \qquad G = EG_{\mathbf{q}} \ltimes T \Rightarrow g_1 = E$$

lattice vec   element of $G_{\mathbf{q}}$

Coset decomposition for inversion: $Ig_1 = \{E|\mathbf{0}\}g_1 I$

coset rep.

$$I|\phi_{\mathbf{R}}\rangle = |\phi_{-\mathbf{R}}\rangle \boxed{\rho(I)}$$

Since there are no other sites, this is exactly U

Conclusion: for s orbitals, U = (1), and for p orbitals, U =(-1)

As we asserted yesterday, for s and p orbitals, $U_I = \begin{pmatrix} +1 & \\ & -1 \end{pmatrix}$

To find little group irreps, plug into the character formula:

Character of h={P,**v**} is given by trace:

$$\mathrm{Tr}\left[V(\mathbf{G})^{-1}U_h\right]e^{-i(P\mathbf{k})\cdot\mathbf{v}},\ P\mathbf{k}=\mathbf{k}+\mathbf{G}$$

Simplifications:

$V(\mathbf{G})=\mathbb{I}$ because atoms at r=0

$\mathbf{v}=0$ because we are only considering inversion

Character table

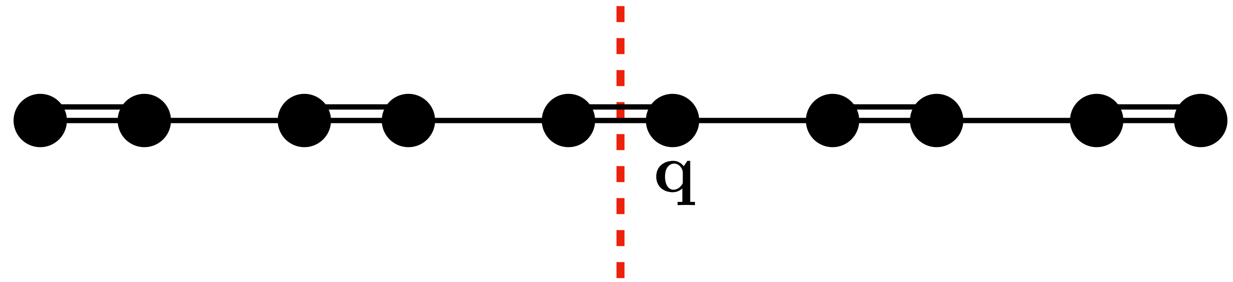
$C_i(-1)$	#	1	-1
A_g	Γ_1^+	1	1
A_u	Γ_1^-	1	-1

At both k=0 and k=π, the character is $\mathrm{Tr}[U_I]=\mathrm{Tr}[\rho(I)]$

For s orbital: $\mathrm{Tr}[U_I]$ = +1 ⇒ A_g

For p orbitals: $\mathrm{Tr}[U_I]$ = -1 ⇒ A_u

Example: band representation of 1D lattice with inversion, atoms at general position



$$G_{\mathbf{q}} = \{E\}$$

$$G = (EG_{\mathbf{q}} \cup IG_{\mathbf{q}}) \ltimes T$$

$$g_1 = E, g_2 = I$$

lattice vec   element of $G_{\mathbf{q}}$

Coset decomposition for inversion:

$$Ig_1 = \{E|\mathbf{0}\}g_2 E$$

$$Ig_2 = \{E|\mathbf{0}\}g_1 E$$

coset rep.

$$I|\phi_{\mathbf{R},1}\rangle = |\phi_{-\mathbf{R},2}\rangle\rho(E)$$

$$I|\phi_{\mathbf{R},2}\rangle = |\phi_{-\mathbf{R},1}\rangle\rho(E)$$

Conclusion: as we asserted yesterday,

$$U_I = \begin{pmatrix} & 1 \\ 1 & \end{pmatrix}$$

To find little group irreps, plug into the character formula:

Character of h={P,**v**} is given by trace:

$$\mathrm{Tr}\left[V(\mathbf{G})^{-1}U_h\right]e^{-i(P\mathbf{k})\cdot\mathbf{v}},\ P\mathbf{k}=\mathbf{k}+\mathbf{G}$$

Simplification:

$$V(\mathbf{G})=\begin{pmatrix} e^{i\mathbf{G}\cdot\mathbf{x}_0} & 0 \\ 0 & e^{-i\mathbf{G}\cdot\mathbf{x}_0}\end{pmatrix}$$

$$\mathrm{Tr}\left[V(\mathbf{G})^{-1}U_h\right]=\mathrm{Tr}\begin{pmatrix} 0 & e^{i\mathbf{G}\cdot\mathbf{x}_0} \\ e^{-i\mathbf{G}\cdot\mathbf{x}_0} & 0\end{pmatrix}=0$$

Character table

$C_i(-1)$	#	1	-1
A_g	Γ_1^+	1	1
A_u	Γ_1^-	1	-1

At both k=0 and k=π, the character is 0

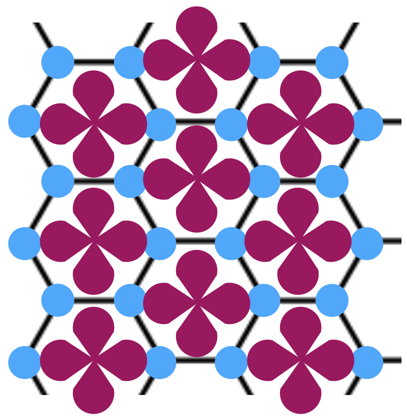
2d rep with zero inversion character: $A_g \oplus A_u$

Part 2: Elementary band representations

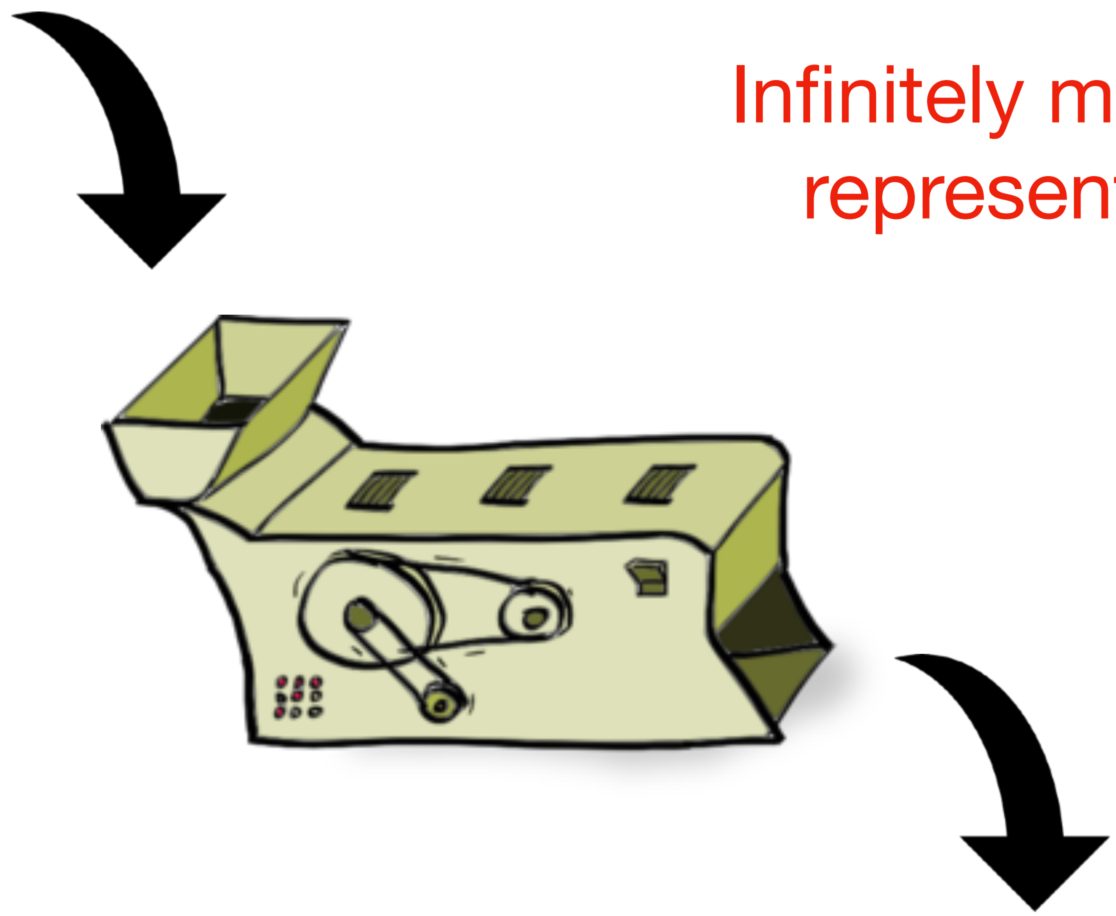
Refs: “Topological quantum chemistry,”
Bradlyn, Elcoro, Cano, Vergniory, Wang, Felser, Aroyo, Bernevig
ArXiv: 1703.02050, Nature 547, 298 — 305 (2017)

“Building blocks of topological quantum chemistry,”
Cano, Bradlyn, Wang, Elcoro, Vergniory, Felser, Aroyo, Bernevig
ArXiv: 1709.01935, PRB 97, 035139 (2018)
Secs II and III

Band representations can describe multiple orbitals in different positions

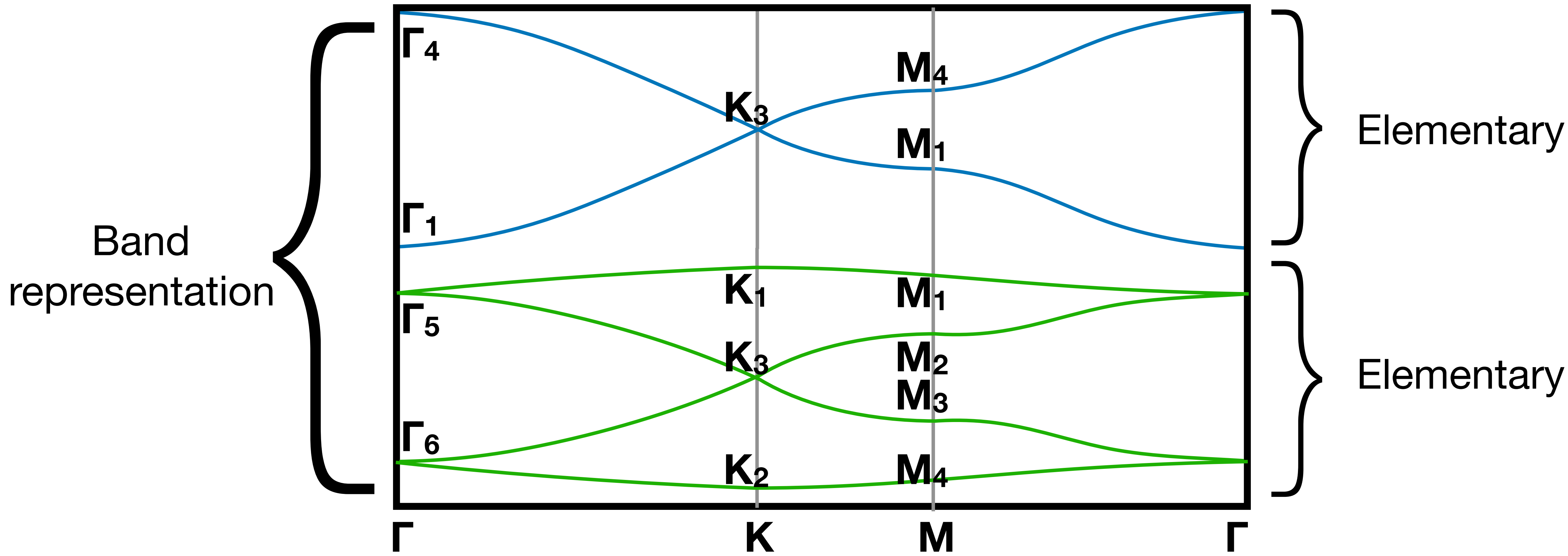


Infinitely many band representations!



Γ_1 Γ_4 Γ_5 Γ_6 K_3 K_3 K_3 M_1 M_1 M_2 M_3 M_4 M_4

Elementary band reps are the building blocks



<u>Elementary</u> band representations do not decompose into sum of band representations

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

$$(\rho_1 \oplus \rho_2) \uparrow G = (\rho_1 \uparrow G) \oplus (\rho_2 \uparrow G)$$

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

$$(\rho \uparrow H) \uparrow G = \rho \uparrow G \qquad K \subset H \subset G$$

⇒ 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 space groups) x (3 max Wyckoff pos.) x (3 irreps) = 2070

Actual:	**no TR**	**TR**
Single-valued irreps (spinless)	3383	3141
Double-valued irreps (spinful)	2263	1616

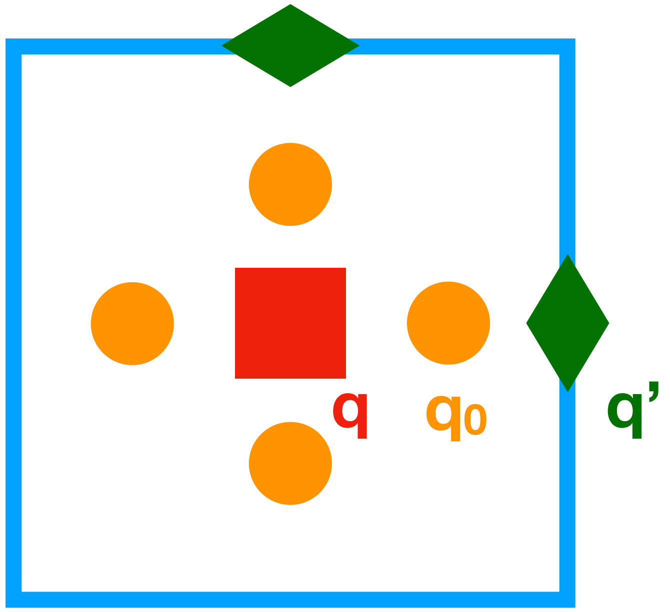
⇒ 10,403 total EBRs

Decomposition into band representations is not unique

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

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

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



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

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

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 $\mathbf{q} = 1/2 \rightarrow -1/2$.

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 $\mathbf{q}=1/2$ 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 $\mathbf{k}=0$ and $\mathbf{k}=\pi$, for each of the irreps of the site-symmetry group. (Hint: $\mathbf{v}=0$ because inversion is a point group operation. But $\mathbf{G}$ is different at $\mathbf{k}=0$ and $\mathbf{k}=\pi$. What irrep appears at $\mathbf{k}=0$? $\mathbf{k}=\pi$?

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 $\mathbf{q}=0$? How does it compare to $\mathbf{q}=\mathbf{x}_0$, $0< \mathbf{x}_0 < 1/2$.

h) Explain why the three band representations are the same. Which are elementary?

Exercises, cont.

Band representation for p4mm.

a) For q=(0,0), what is the site-symmetry group? What is ρ(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 ρ(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: $hg_\alpha = \{E|\mathbf{t}\}g_\beta g, \mathbf{t} = h\mathbf{q}_\alpha - \mathbf{q}_\beta$
Hint: act with both sides on the site **q**. Also recall $\mathbf{q}_\alpha \equiv g_\alpha \mathbf{q}$.

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

c) Recalling, P**R** + **t** = **R'**, prove yesterday's equation for the same symmetry operation:

$$P(\mathbf{R} + \mathbf{q}_\alpha) + \mathbf{v} = \mathbf{R}' + \mathbf{q}_\beta$$