Tight binding models from band representations

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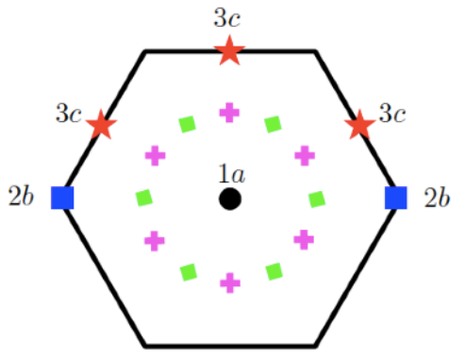
Part 0: Review of band representations

BANDREP

http://www.cryst.ehu.es/cgi-bin/cryst/programs/bandrep.pl

- Input: orbital, Wyckoff position, space group
- Output:
  - irreps at high-symmetry points
  - compatibility relations
  - band connectivity

Example: p6mm



Bilbao Crystallographic Server → BANDREP Help

Elementary band-representations without time-reversal symmetry of the Double Space Group *P6mm* (No. 183)

The first row shows the Wyckoff position from which the band representation is induced.
In parentheses, the symbol of the point group isomorphic to the site-symmetry group.

The second row gives the symbol ρ↑G, where ρ is the irrep of the site-symmetry group.
In parentheses, the dimension of the representation.

The output shows the decomposition of the band representations into irreps of the little groups of the given k-vectors in the first column.
In parentheses, the dimensions of the representations.

Minimal set of paths and compatibility relations to analyse the connectivity

Show all types of k-vectors

Wyckoff pos.	1a(6*mm*)	1a(6*mm*)	1a(6*mm*)	1a(6*mm*)	1a(6*mm*)	1a(6*mm*)	...	2b(3*m*)
Band-Rep.	$A_1\uparrow G(1)$	$A_2\uparrow G(1)$	$B_1\uparrow G(1)$	$B_2\uparrow G(1)$	$E_1\uparrow G(2)$	$E_2\uparrow G(2)$		$\bar{E}_1\uparrow G(4)$
Decomposable\ Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable	Indecomposable		Decomposable
A:(0,0,1/2)	$A_1(1)$	$A_2(1)$	$A_4(1)$	$A_3(1)$	$A_6(2)$	$A_5(2)$		$\bar{A}_8(2) \oplus \bar{A}_9(2)$
Γ:(0,0,0)	$\Gamma_1(1)$	$\Gamma_2(1)$	$\Gamma_4(1)$	$\Gamma_3(1)$	$\Gamma_6(2)$	$\Gamma_5(2)$		$\bar{\Gamma}_8(2) \oplus \bar{\Gamma}_9(2)$
H:(1/3,1/3,1/2)	$H_1(1)$	$H_2(1)$	$H_2(1)$	$H_1(1)$	$H_3(2)$	$H_3(2)$		$\bar{H}_4(1) \oplus \bar{H}_5(1) \oplus \bar{H}_6(2)$
K:(1/3,1/3,0)	$K_1(1)$	$K_2(1)$	$K_2(1)$	$K_1(1)$	$K_3(2)$	$K_3(2)$		$\bar{K}_4(1) \oplus \bar{K}_5(1) \oplus \bar{K}_6(2)$
L:(1/2,0,1/2)	$L_1(1)$	$L_2(1)$	$L_4(1)$	$L_3(1)$	$L_3(1) \oplus L_4(1)$	$L_1(1) \oplus L_2(1)$		$2\,\bar{L}_5(2)$
M:(1/2,0,0)	$M_1(1)$	$M_2(1)$	$M_4(1)$	$M_3(1)$	$M_3(1) \oplus M_4(1)$	$M_1(1) \oplus M_2(1)$		$2\,\bar{M}_5(2)$

Compatibility relations constrain connectivity

Compatibility Relations
$GM_1(1) \rightarrow LD_1(1)$
$GM_2(1) \rightarrow LD_2(1)$
$GM_3(1) \rightarrow LD_1(1)$
$GM_4(1) \rightarrow LD_2(1)$
$GM_5(2) \rightarrow LD_1(1) \oplus LD_2(1)$
$GM_6(2) \rightarrow LD_1(1) \oplus LD_2(1)$
$\overline{GM_7}(2) \rightarrow \overline{LD_3}(1) \oplus \overline{LD_4}(1)$
$\overline{GM_8}(2) \rightarrow \overline{LD_3}(1) \oplus \overline{LD_4}(1)$
$\overline{GM_9}(2) \rightarrow \overline{LD_3}(1) \oplus \overline{LD_4}(1)$

Compatibility Relations
$K_1(1) \rightarrow LD_1(1)$
$K_2(1) \rightarrow LD_2(1)$
$K_3(2) \rightarrow LD_1(1) \oplus LD_2(1)$
$\overline{K_4}(1) \rightarrow \overline{LD_3}(1)$
$\overline{K_5}(1) \rightarrow \overline{LD_4}(1)$
$\overline{K_6}(2) \rightarrow \overline{LD_3}(1) \oplus \overline{LD_4}(1)$

Compatibility Relations
$M_1(1) \rightarrow LD_1(1)$
$M_2(1) \rightarrow LD_2(1)$
$M_3(1) \rightarrow LD_1(1)$
$M_4(1) \rightarrow LD_2(1)$
$\overline{M_5}(2) \rightarrow \overline{LD_3}(1) \oplus \overline{LD_4}(1)$

Compatibility Relations
$M_1(1) \rightarrow SM_1(1)$
$M_2(1) \rightarrow SM_2(1)$
$M_3(1) \rightarrow SM_2(1)$
$M_4(1) \rightarrow SM_1(1)$
$\overline{M_5}(2) \rightarrow \overline{SM_3}(1) \oplus \overline{SM_4}(1)$

Compatibility Relations
$GM_1(1) \rightarrow SM_1(1)$
$GM_2(1) \rightarrow SM_2(1)$
$GM_3(1) \rightarrow SM_2(1)$
$GM_4(1) \rightarrow SM_1(1)$
$GM_5(2) \rightarrow SM_1(1) \oplus SM_2(1)$
$GM_6(2) \rightarrow SM_1(1) \oplus SM_2(1)$
$\overline{GM_7}(2) \rightarrow \overline{SM_3}(1) \oplus \overline{SM_4}(1)$
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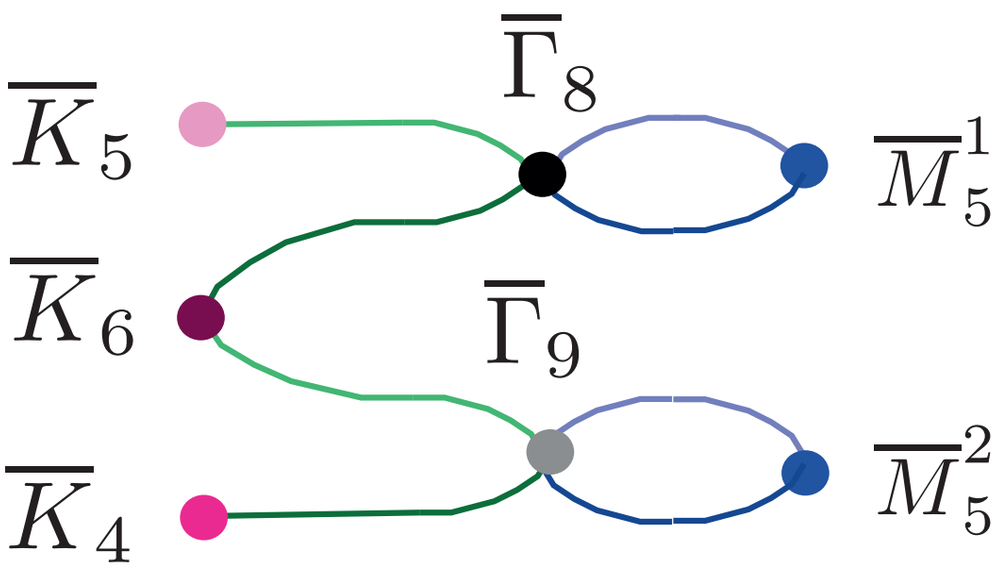
$\overline{GM_9}(2) \rightarrow \overline{SM_3}(1) \oplus \overline{SM_4}(1)$

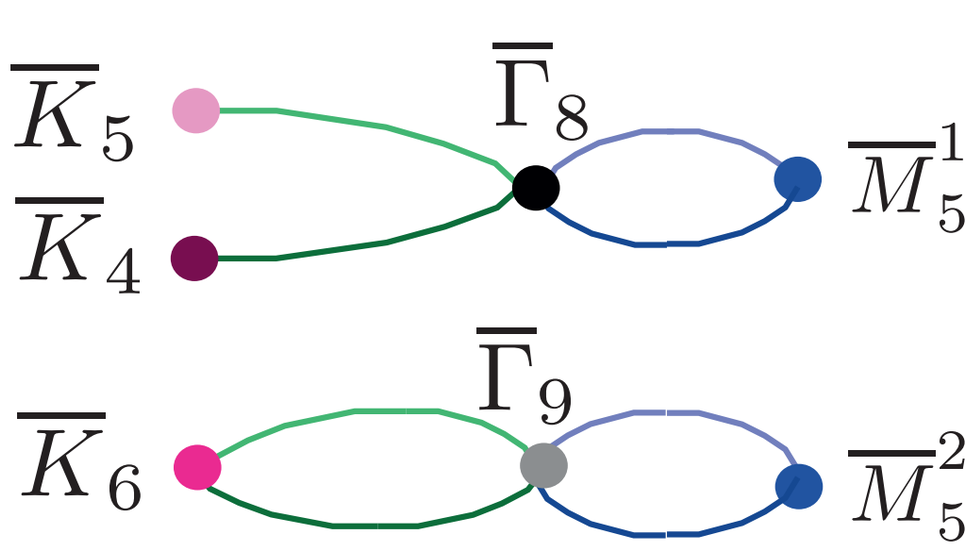
Compatibility relations constrain connectivity

2 possible connectivities for the band rep $\overline{E}_1\uparrow G(4)$

Connected



Disconnected



“decomposable” connectivity indicated in BANDREP

Main point: real space symmetry highly constrains band connectivity

Goals of this lecture

- Given Wyckoff position and orbital, write band rep matrices
- Build a tight-binding model with symmetries

Part 1: Bloch's theorem

For electrons in a perfect crystal, there is a basis of wavefunctions with the properties:

- *Each of these wavefunctions is an energy eigenstate*
- *Each of these wavefunctions is a Bloch wave, meaning that this wavefunction ψ can be written in the form*

$$\psi(\mathbf{r}) = \mathrm{e}^{\mathrm{i}\mathbf{k}\cdot\mathbf{r}} u(\mathbf{r})$$

where u has the same periodicity as the atomic structure of the crystal.

https://en.wikipedia.org/wiki/Bloch_wave#Proof_of_Bloch's_theorem

Proof of Bloch's theorem
1. define simultaneous eigenstates of H, T

$$H(\mathbf{r}+\mathbf{R}) = H(\mathbf{r}) \qquad \mathbf{R} = n_1\mathbf{e}_1 + n_2\mathbf{e}_2 + n_3\mathbf{e}_3, n_i \in \mathbb{Z}$$

Hamiltonian commutes with translations: $[H, T_{\mathbf{e}_i}] = 0$

Simultaneous eigenstates:

$$T_{\mathbf{e}_i}\psi_{n,\mathbf{k}} = e^{-2\pi i k_i}\psi_{n,\mathbf{k}} \qquad \mathbf{k} \equiv k_1\mathbf{g}_1 + k_2\mathbf{g}_2 + k_3\mathbf{g}_3$$

$$H\psi_{n,\mathbf{k}} = E_{n,\mathbf{k}}\psi_{n,\mathbf{k}} \qquad \mathbf{e}_i \cdot \mathbf{g}_j = 2\pi\delta_{ij}$$

$$\Rightarrow \psi_{n,\mathbf{k}}(\mathbf{r}-\mathbf{R}) = T_{\mathbf{e}_1}^{n_1} T_{\mathbf{e}_2}^{n_2} T_{\mathbf{e}_3}^{n_3} \psi_{n,\mathbf{k}}(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{R}}\psi_{n,\mathbf{k}}$$

Proof of Bloch's theorem
2. construct real space periodic function

$$u_{\mathbf{k}}(\mathbf{r}) = e^{-i\mathbf{k}\cdot\mathbf{r}}\psi_{\mathbf{k}}(\mathbf{r})$$

$$\begin{aligned} u_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) &= e^{-i\mathbf{k}\cdot(\mathbf{r}+\mathbf{R})}\psi_{\mathbf{k}}(\mathbf{r}+\mathbf{R}) \\ &= e^{-i\mathbf{k}\cdot(\mathbf{r}+\mathbf{R})}e^{i\mathbf{k}\cdot\mathbf{R}}\psi_{\mathbf{k}}(\mathbf{r}) \\ &= e^{-i\mathbf{k}\cdot\mathbf{r}}\psi_{\mathbf{k}}(\mathbf{r}) \\ &= u_{\mathbf{k}}(\mathbf{r}) \end{aligned}$$

u has periodicity of lattice, not periodicity of BZ

ψ has periodicity of BZ, not periodicity of lattice

Should we use *u* or *ψ*?

- *u* is the natural way to define the Berry phase

$\nabla_{\mathbf{k}} u_{\mathbf{k}}$ is well-defined and periodic

$$\nabla_{\mathbf{k}} \psi_{\mathbf{k}} = \nabla (e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}) = e^{i\mathbf{k}\cdot\mathbf{r}} (\nabla_{\mathbf{k}} u_{\mathbf{k}} + i\mathbf{r} u_{\mathbf{k}})$$

blows up away from origin

- stay tuned for Barry's lectures

Part 2: tight-binding model formalism

Following notes by Yusufaly, Vanderbilt and Coh, available at:

http://www.physics.rutgers.edu/pythtb/_downloads/pythtb-formalism.pdf

Tight-binding degrees of freedom

Atoms located at positions: $\mathbf{r}_\alpha$

Each atom has orbitals labelled by j = 1, …, n

$$\phi_{\mathbf{R},\alpha,j}(\mathbf{r}) = \varphi_{\alpha,j}(\mathbf{r} - \mathbf{R} - \mathbf{r}_\alpha)$$

unit cell atom orbital

assume orthonormality: $\langle \phi_{\mathbf{R},\alpha,j} | \phi_{\mathbf{R}',\beta,i} \rangle = \delta_{R,\mathbf{R}'}\delta_{\alpha,\beta}\delta_{ij}$

position operator: $\langle \phi_{\mathbf{R},\alpha,j} | \mathbf{r} | \phi_{\mathbf{R}',\beta,i} \rangle = (\mathbf{R} + \mathbf{r}_\alpha)\delta_{R,\mathbf{R}'}\delta_{\alpha,\beta}\delta_{ij}$

Tight-binding Hamiltonian

$$H_{\alpha i,\beta j}(\mathbf{R}) \equiv \langle \phi_{\mathbf{R}',\alpha,i} | H | \phi_{\mathbf{R}'+R,\beta,j} \rangle = \langle \phi_{0,\alpha,i} | H | \phi_{\mathbf{R},\beta,j} \rangle$$

Translation invariance ⇒ only specify atoms/orbitals and R

Two natural choices of Fourier transform

Choice 1:

$$|\chi^{\mathbf{k}}_{\alpha,j}\rangle = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot(\mathbf{R}+\mathbf{r}_\alpha)}|\phi_{\mathbf{R},\alpha,j}\rangle$$

$$H^{\mathbf{k}}_{\alpha i,\beta j} \equiv \langle\chi^{\mathbf{k}}_{\alpha i}|H|\chi^{\mathbf{k}}_{\beta j}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{r}_\alpha+\mathbf{r}_\beta)} H_{\alpha i,\beta j}(\mathbf{R})$$

Choice 2:

$$|\tilde{\chi}^{\mathbf{k}}_{\alpha,j}\rangle = \sum_{\mathbf{k}} e^{i\mathbf{k}\cdot\mathbf{R}}|\phi_{\mathbf{R},\alpha,j}\rangle$$

$$\tilde{H}^{\mathbf{k}}_{\alpha i,\beta j} \equiv \langle\tilde{\chi}^{\mathbf{k}}_{\alpha i}|H|\tilde{\chi}^{\mathbf{k}}_{\beta j}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} H_{\alpha i,\beta j}(\mathbf{R})$$

Note: only different if more than one site per cell!

Pros/cons of Fourier transform choices

Choice 2:

$$\tilde{H}^{\mathbf{k}}_{\alpha i,\beta j} \equiv \langle \tilde{\chi}^{\mathbf{k}}_{\alpha i} | H | \tilde{\chi}^{\mathbf{k}}_{\beta j} \rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} H_{\alpha i,\beta j}(\mathbf{R})$$

Hamiltonian is periodic in Brillouin zone

Choice 1:

$$H^{\mathbf{k}}_{\alpha i,\beta j} \equiv \langle \chi^{\mathbf{k}}_{\alpha i} | H | \chi^{\mathbf{k}}_{\beta j} \rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot(\mathbf{R}-\mathbf{r}_\alpha+\mathbf{r}_\beta)} H_{\alpha i,\beta j}(\mathbf{R})$$

Hamiltonian is not periodic in Brillouin zone

Pro: Symmetries without translations are k-independent (will prove)

Since we are mostly concerned with symmetries, we use Choice 1 in these lectures!!!

Choice 2: Periodicity of Hamiltonian

Define diagonal matrix: $V(\mathbf{k})_{\alpha i,\beta j} = \delta_{\alpha\beta}\delta_{ij}e^{i\mathbf{k}\cdot\mathbf{r}_\alpha}$

$$H^{\mathbf{k}+\mathbf{G}}_{\alpha i,\beta j} = e^{i\mathbf{G}\cdot(\mathbf{r}_\beta-\mathbf{r}_\alpha)}H^{\mathbf{k}}_{\alpha i,\beta j} = \left[V(\mathbf{G})^{-1}H^{\mathbf{k}}V(\mathbf{G})\right]_{\alpha i,\beta j}$$

Notes:

H is not periodic in BZ, but

H(k) and H(k+G) have same eigenvalues (of course)

Fourier conventions: analogy to *u* and ψ

Hamiltonians generate eigenvalue equations:

$$H^{\mathbf{k}}_{\alpha i,\beta j} C^{n\mathbf{k}}_{\beta j} = E_{n\mathbf{k}} C^{n\mathbf{k}}_{\alpha i}$$

$$\tilde{H}^{\mathbf{k}}_{\alpha i,\beta j} \tilde{C}^{n\mathbf{k}}_{\beta j} = E_{n\mathbf{k}} \tilde{C}^{n\mathbf{k}}_{\alpha i}$$

Eigenstates:

$$\sum_{\alpha i} C^{n\mathbf{k}}_{\alpha i} |\chi^{\mathbf{k}}_{\alpha i}\rangle$$

$$\sum_{\alpha i} \tilde{C}^{n\mathbf{k}}_{\alpha i} |\tilde{\chi}^{\mathbf{k}}_{\alpha i}\rangle$$

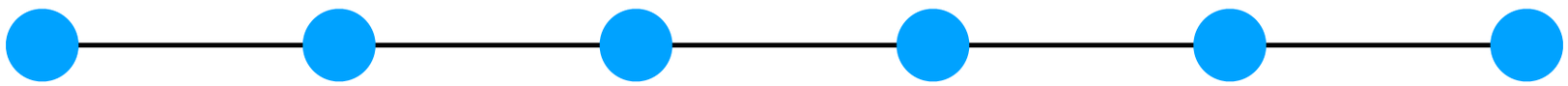
$$\tilde{C}^{n,\mathbf{k}+\mathbf{G}}_{\alpha i} = \tilde{C}^{n,\mathbf{k}}_{\alpha i} \qquad \Rightarrow \text{BZ periodic, like } \psi$$

$$C^{n,\mathbf{k}+\mathbf{G}}_{\alpha i} = e^{-i\mathbf{G}\cdot\mathbf{r}_\alpha} C^{n,\mathbf{k}}_{\alpha i} \qquad \Rightarrow \text{not BZ periodic, like } u$$

Using Choice 1 instead of Choice 2 is similar to using *u* instead of ψ

(which we argued earlier was more natural for topological applications)

Example 1: atoms in 1d

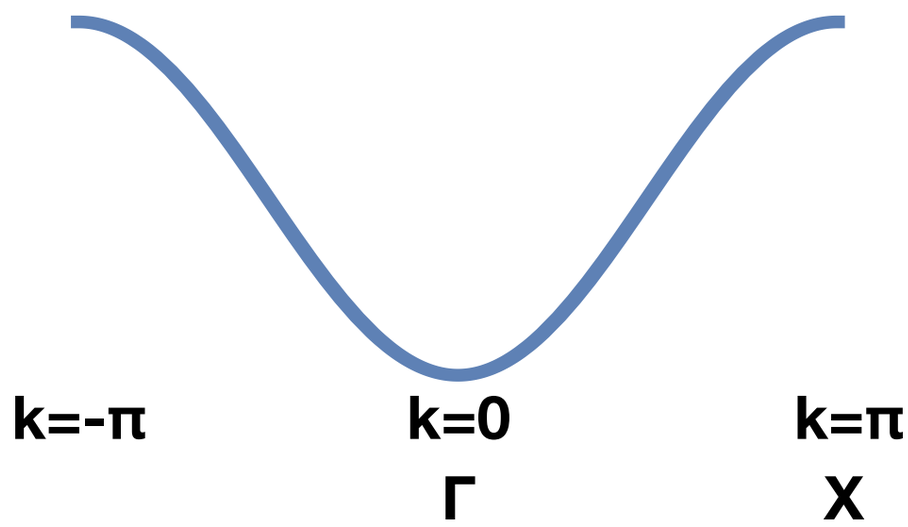


1 orbital/site ⇒ trivial subscripts: $\mathbf{r}_\alpha = \mathbf{r}_1 = \mathbf{0} \quad i = 1$

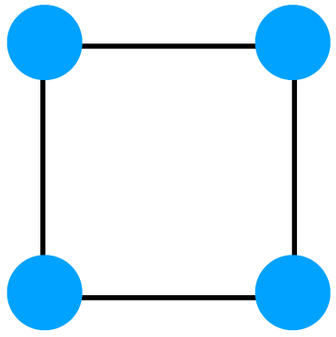
$$H(\mathbf{R} = \pm\hat{x}) = -t$$

$$H(\mathbf{R} \neq \pm\hat{x}) = 0$$

$$H^{\mathbf{k}} = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} H(\mathbf{R}) = -t(e^{i\mathbf{k}\cdot\hat{x}} + e^{-i\mathbf{k}\cdot\hat{x}}) = -2t\cos k$$



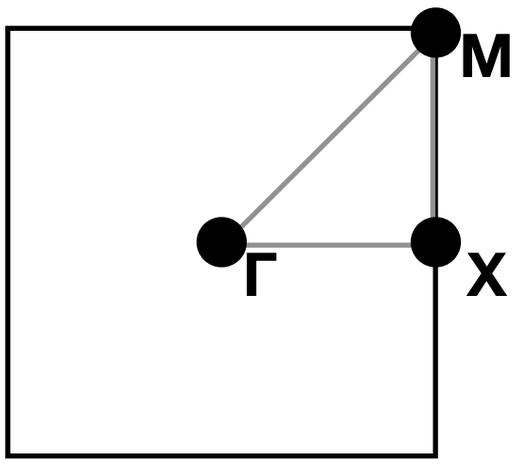
Example 2: square lattice

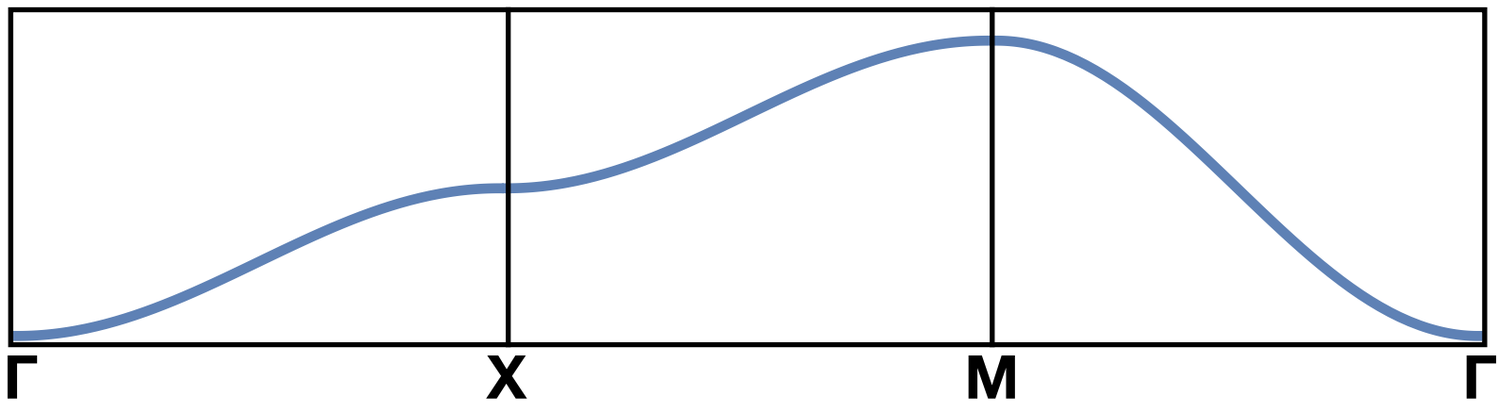


$$H(\mathbf{R}) = \begin{cases} -t & \text{if } \mathbf{R} = \pm\hat{x}, \pm\hat{y} \\ 0 & \text{else} \end{cases}$$

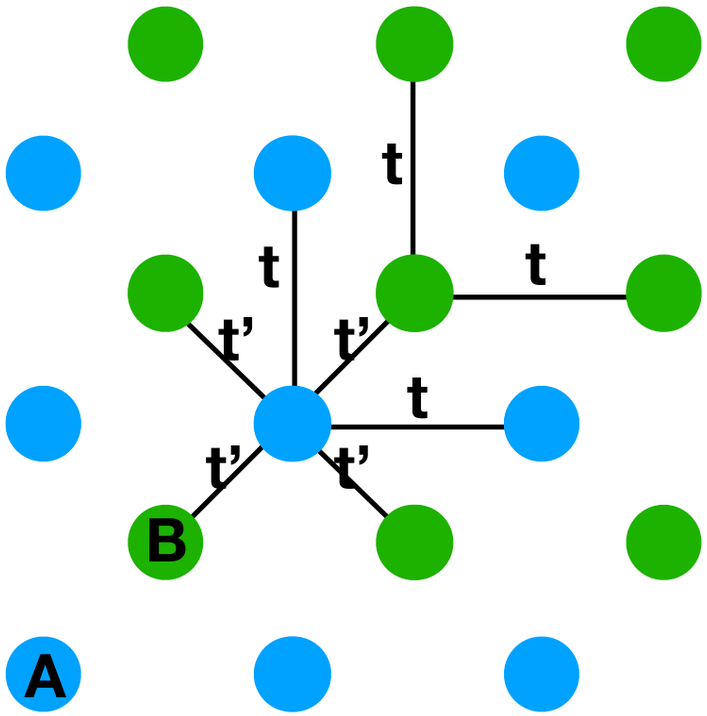
$$H^{\mathbf{k}} = -2t(\cos k_x + \cos k_y)$$

How to plot 2d spectrum? identify high-symmetry path





Example 3: interpenetrating square lattices



$$\mathbf{r}_A = (0,0)$$

$$\mathbf{r}_B = (1/2,1/2)$$

only one orbital/site ⇒ i = 1

$$H_{AA}(\mathbf{0}) = \mu_A$$

$$H_{BB}(\mathbf{0}) = \mu_B$$

$$H_{AA}(\pm\hat{x}) = H_{AA}(\pm\hat{y}) = H_{BB}(\pm\hat{x}) = H_{BB}(\pm\hat{y}) = -t$$

$$H_{AB}(\mathbf{0}) = H_{AB}(-\hat{x}) = H_{AB}(-\hat{x}-\hat{y}) = H_{AB}(-\hat{y}) = -t'$$

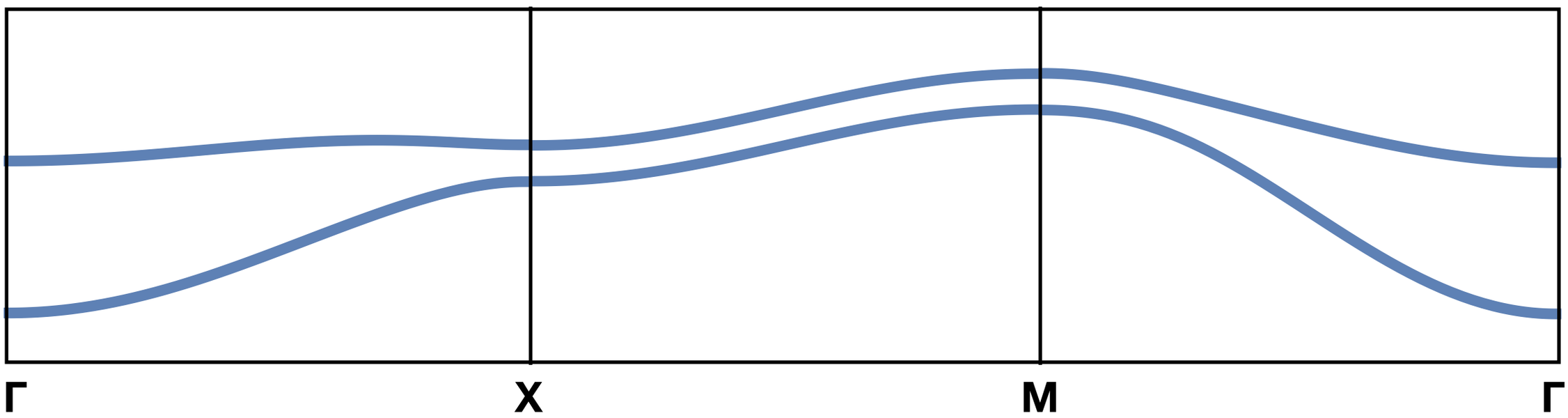
label by **R**, not $\mathbf{r}_{AB}$

Example 3: interpenetrating square lattices, cont.

$$H^{\mathbf{k}}_{AA} = -2t(\cos k_x + \cos k_y) + \mu_A$$

$$H^{\mathbf{k}}_{BB} = -2t(\cos k_x + \cos k_y) + \mu_B$$

$$\begin{aligned} H^{\mathbf{k}}_{AB} &= -t'(e^{i\mathbf{k}\cdot(\mathbf{0}+\mathbf{r}_B)} + e^{i\mathbf{k}\cdot(-\hat{x}+\mathbf{r}_B)} + e^{i\mathbf{k}\cdot(-\hat{x}-\hat{y}+\mathbf{r}_B)} + e^{i\mathbf{k}\cdot(-\hat{y}+\mathbf{r}_B)}) \\ &= -t'(e^{i\mathbf{k}\cdot(\frac{1}{2},\frac{1}{2})} + e^{i\mathbf{k}\cdot(-\frac{1}{2},\frac{1}{2})} + e^{i\mathbf{k}\cdot(-\frac{1}{2},-\frac{1}{2})} + e^{i\mathbf{k}\cdot(\frac{1}{2},-\frac{1}{2})}) \\ &= -4t' \cos\frac{k_x}{2} \cos\frac{k_y}{2} \end{aligned}$$



Part 3: tight-binding symmetries

How do crystal symmetries act on tight-binding states?

$$g = \{P|\mathbf{v}\} \qquad\qquad \mathbf{r} \to P\mathbf{r} + \mathbf{v}$$

point group element translation

Action on TB states: $g|\phi_{\mathbf{R},\alpha i}\rangle = [U_g]_{\beta j,\alpha i}|\phi_{\mathbf{R}',\beta j}\rangle$

R', β fixed by spatial rotation: $P(\mathbf{R} + \mathbf{r}_\alpha) + \mathbf{v} = \mathbf{R}' + \mathbf{r}_\beta$

U describes orbital rotation ⇒ U is independent of R (will prove)

How do crystal symmetries act on Fourier-transformed TB basis?

$$
\begin{aligned}
g|\chi^{\mathbf{k}}_{\alpha i}\rangle &= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot(\mathbf{R}+\mathbf{r}_\alpha)} g|\phi_{\mathbf{R},\alpha i}\rangle \\
&= \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot(\mathbf{R}+\mathbf{r}_\alpha)} |\phi_{\mathbf{R}',\beta j}\rangle [U_g]_{\beta j,\alpha i} \\
&= \sum_{\mathbf{R}} e^{i(P\mathbf{k})\cdot(P(\mathbf{R}+\mathbf{r}_\alpha))} |\phi_{\mathbf{R}',\beta j}\rangle [U_g]_{\beta j,\alpha i} \\
&= \sum_{\mathbf{R}} e^{i(P\mathbf{k})\cdot(\mathbf{R}'+\mathbf{r}_\beta-\mathbf{v})} |\phi_{\mathbf{R}',\beta j}\rangle [U_g]_{\beta j,\alpha i} \\
&= |\chi^{P\mathbf{k}}_{\beta j}\rangle [U_g]_{\beta j,\alpha i} e^{-i(P\mathbf{k})\cdot\mathbf{v}}
\end{aligned}
$$

Proof (promised earlier) that if v=0, then g is k-independent

More generally, g splits into k-independent matrix and k-dependent phase

How does the tight-binding Hamiltonian transform under symmetries?

Real space: $gHg^{-1} = H$

Momentum space:
$$H^{\mathbf{k}}_{\alpha i,\beta j} \equiv \langle \chi^{\mathbf{k}}_{\alpha i} | H | \chi^{\mathbf{k}}_{\beta j} \rangle = \langle \chi^{\mathbf{k}}_{\alpha i} | g H g^{-1} | \chi^{\mathbf{k}}_{\beta j} \rangle$$

Expand RHS:
$$= \langle \chi^{\mathbf{k}}_{\alpha i} | g | \chi^{\mathbf{k}'}_{\delta l} \rangle \langle \chi^{\mathbf{k}'}_{\delta l} | H | \chi^{\mathbf{k}''}_{\gamma m} \rangle \langle \chi^{\mathbf{k}''}_{\gamma m} | g^{-1} | \chi^{\mathbf{k}}_{\beta j} \rangle$$

$$= \left([U_g]_{\alpha i,\delta l} \delta_{P\mathbf{k}',\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{v}} \right) \left(\delta_{\mathbf{k}',\mathbf{k}''} H^{\mathbf{k}'}_{\delta l,\gamma m} \right) \left([U_g^{-1}]_{\gamma m,\beta j} \delta_{P^{-1}\mathbf{k},\mathbf{k}''} e^{-i\mathbf{k}''\cdot(-P^{-1}\mathbf{v})} \right)$$

Conclude:
$$H^{\mathbf{k}}_{\alpha i,\beta j} = \left[U_g H^{P^{-1}\mathbf{k}} U_g^{-1} \right]_{\alpha i,\beta j}$$

The k-independent matrix U determines symmetry of Hamiltonian (even in non-symmorphic group!!)

How to find little group irreps

Little group: $G_{\mathbf{k}} = \{g | g\mathbf{k} = \mathbf{k} + \mathbf{G}\}$

In our gauge, U_g does not commute with H^k:

$$U_g H^{\mathbf{k}} U_g^{-1} = H^{\mathbf{k}+\mathbf{G}} = V(\mathbf{G})^{-1} H^{\mathbf{k}} V(\mathbf{G})$$

Recall: $V(\mathbf{k})_{\alpha i,\beta j} = \delta_{\alpha\beta}\delta_{ij} e^{i\mathbf{k}\cdot\mathbf{r}_\alpha}$

Instead: $[V(\mathbf{G})U_g, H^{\mathbf{k}}] = 0$

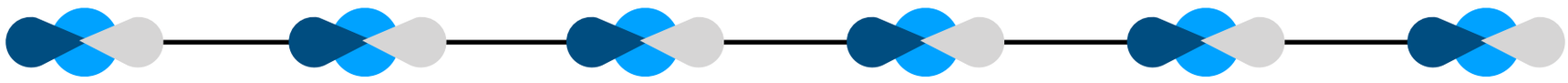
Can simultaneously diagonalize H^k and $V(G)U_g$ (not U_g)

Little group characters from eigenvalues of $V(G)U_g e^{-i(Pk).v}$

(This must be the case, otherwise little group irreps would be k-independent!!)

Note: G is different for different choices of g

Example 1: 1d chain with inversion, s and p orbitals



What is U? inversion does not mix orbitals ⇒ diagonal

$$U = \sigma_z \quad \Rightarrow \quad H^{\mathbf{k}} = \sigma_z H^{-\mathbf{k}} \sigma_z$$

$$H^k = \begin{pmatrix} \mu_s & 0 \\ 0 & \mu_p \end{pmatrix} + \begin{pmatrix} -t_s & 0 \\ 0 & -t_p \end{pmatrix} \cos k + \begin{pmatrix} 0 & -it_{sp} \\ it_{sp} & 0 \end{pmatrix} \sin k + \dots$$

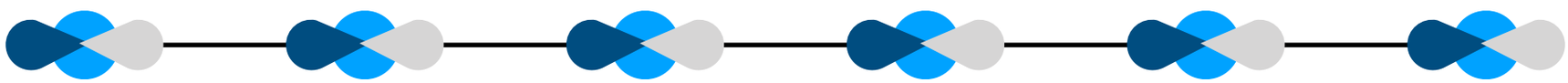
onsite — nearest neighbor, same orbital — nearest neighbor, different orbital orbital

How to implement in real space?

$$H_{ss(pp)}(\hat{x}) = H_{ss(pp)}(-\hat{x}) \qquad H_{sp}(\hat{x}) = -H_{sp}(-\hat{x})$$

Example 1: 1d chain with inversion, s and p orbitals

Compute inversion eigenvalues



$$H^{\Gamma} = \frac{1}{2}(\mu_s - \mu_p - t_s + t_p)\sigma_z + (\cdots)\mathbb{I} + \ldots$$

$$H^{X} = \frac{1}{2}(\mu_s - \mu_p + t_s - t_p)\sigma_z + (\cdots)\mathbb{I} + \ldots$$

$$U_g = \sigma_z \qquad V(\mathbf{k}) = \mathbb{I}$$

Inversion eigenvalues determined by sign of: $(\mu_s - \mu_p) \pm (-t_s + t_p)$

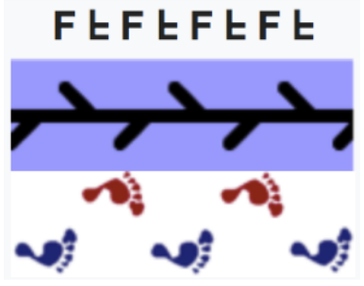
Four possibilities for inversion eigenvalue of lower band: ++, +-, -+, --
Upper band always opposite of lower: --, -+, +-, ++

Can understand from band representations
Four possibilities are four different EBRs

Example 2: pg

(Non-symmorphic) group generated by {m_y | ½ 0}

$$\mathbf{r}_1 = 0, \mathbf{r}_2 = 1/2$$



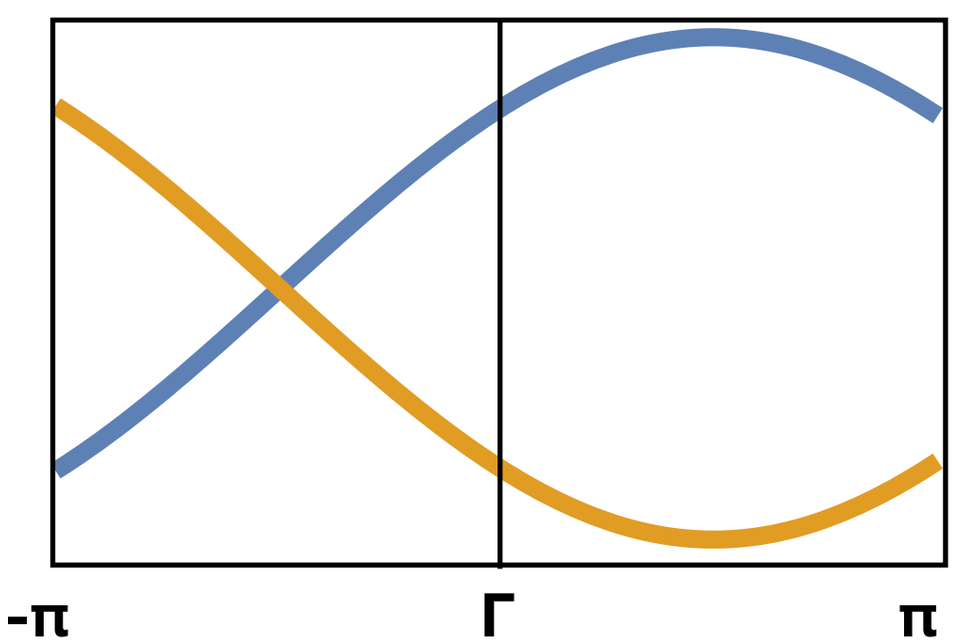
"Frieze" group

What is U? glide exchanges orbitals $U_g = \sigma_x$ $\sigma_x H^k \sigma_x = H^k$

$$H^k = \mu \mathbb{I} + (t \cos \frac{k}{2} + t' \sin \frac{k}{2}) \sigma_x + \dots$$

- both sites have same chemical potential!
- two types of nearest neighbor hopping

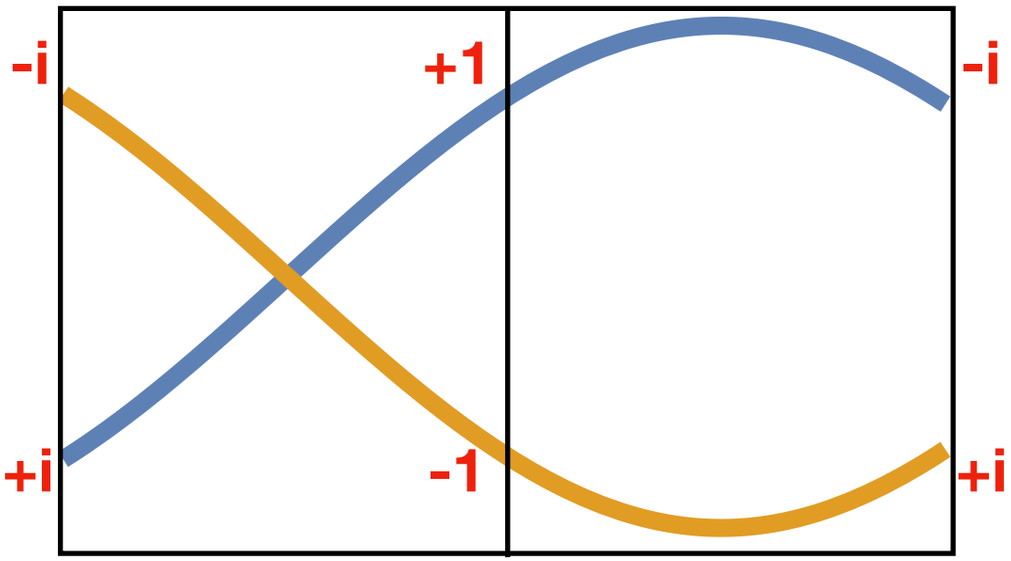
Spectrum: t = t' = 1



Example 2: pg

Compute eigenvalues

$$H^k = \mu\mathbb{I} + (t\cos\frac{k}{2} + t'\sin\frac{k}{2})\sigma_x$$



Band crossing is required!!

Recall: Little group characters from eigenvalues of $V(G)U_g e^{-i(Pk).v}$, where Pk = k+G

$$U_g = \sigma_x$$

$$\mathbf{G} = 0 \Rightarrow V(0) = \mathbb{I}$$

$$e^{-i(Pk)v} = e^{-ik/2}$$

At k, matrix form of glide:

$$\sigma_x e^{-ik/2}$$

Exercises

1. Inversion symmetry in 1d with atoms at the general position. Consider a 1d chain of atoms with two sites per cell at $x = \pm x_0$, invariant under inversion symmetry.

a) What is the matrix form for inversion symmetry?

b) Construct a tight-binding model.

c) Show that the tight-binding Hamiltonian is identical to that for s and p orbitals at x=0 after a basis transformation.

d) What happens when $x_0 = 1/4$?

2. Glide with time-reversal. Consider *pg*, generated by the glide, $\{m_y|1/2, 0\}$.

a) Why is the term $\cos(k)\sigma_x$ forbidden? Hint: what is V(G)?

b) How does time reversal change the band structure? (Time-reversal is implemented by complex conjugation and k → -k.)

c) Bonus: what if SOC is included? Hint: see "Hourglass fermions," by Wang, Alexandradinata, Cava, Bernevig, Arxiv:1602.05585, Nature 532,189-194 (2016)

3. Rectangular lattice. Consider a rectangular lattice of s orbitals, without C_4 symmetry.

a) What extra terms can be added to the Hamiltonian with C_4 symmetry?

b) Along which path should the spectrum be plotted to see all high-symmetry lines?

4. k-independence. Prove that when there is only one atom (perhaps with many orbitals) in the unit cell, then there exists a choice of origin such that the little group irreps are k-independent.