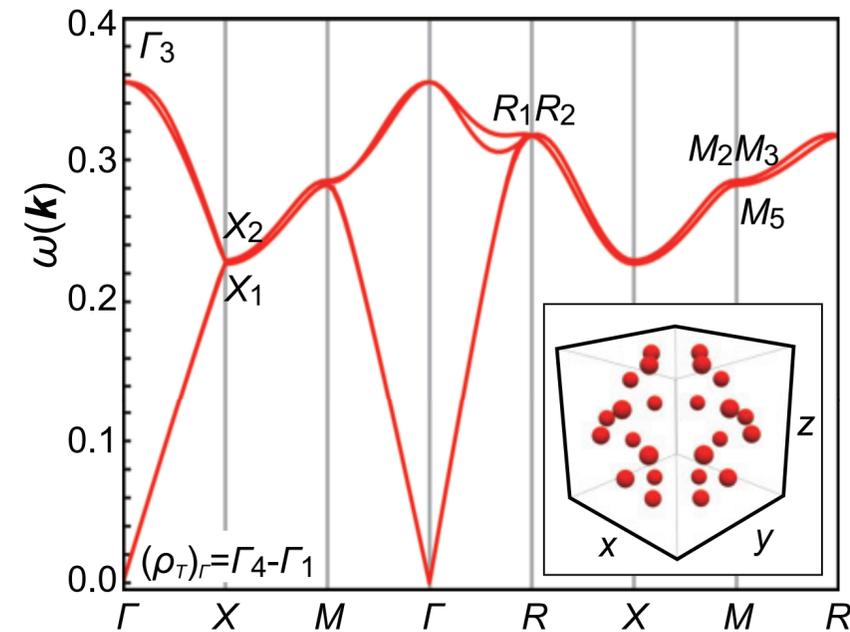
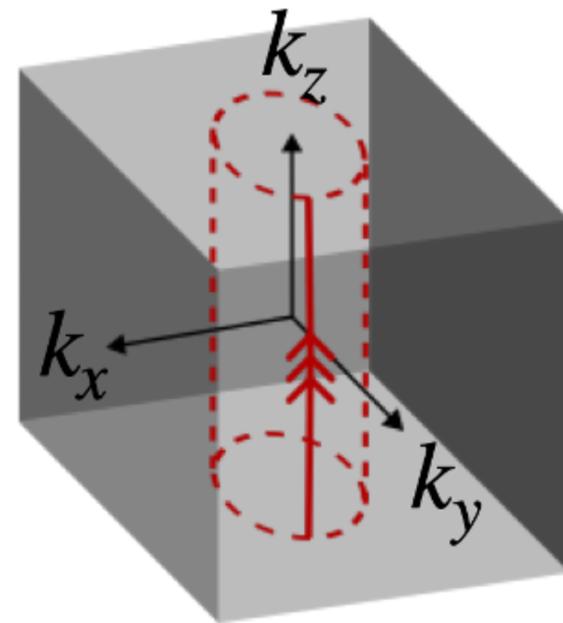


Computing Topological Invariants for 3D Photonic Crystals

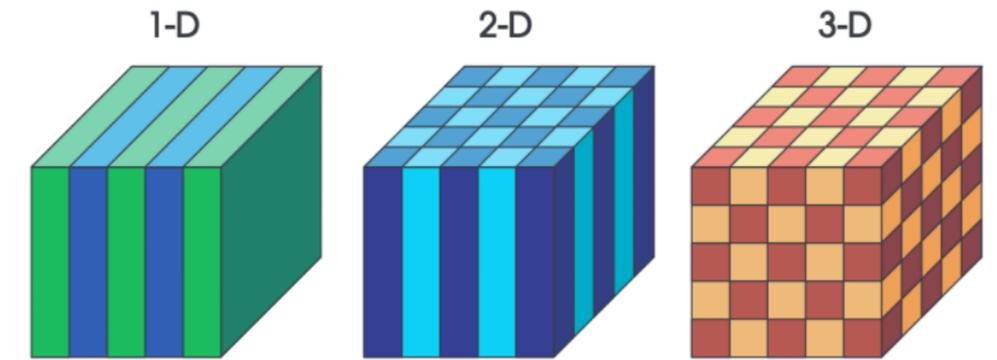


Barry Bradlyn
University of Illinois at Urbana-Champaign

Motivation: Modeling Topological Photonic Crystals

- Periodic dielectric material $\epsilon_{\mu\nu}(\mathbf{r} + \mathbf{a}) = \epsilon_{\mu\nu}(\mathbf{r})$

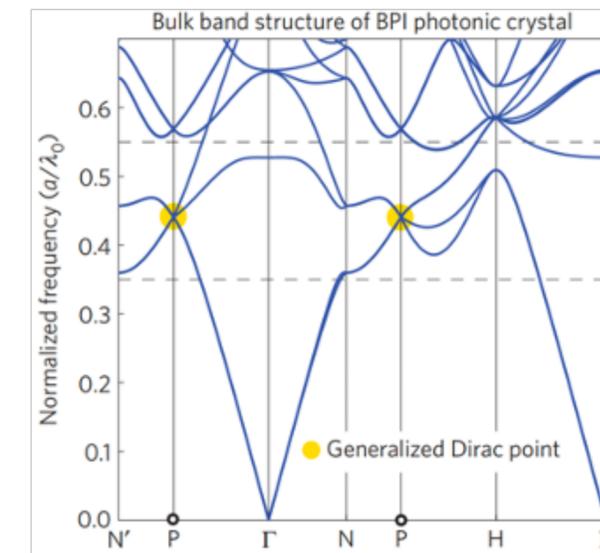
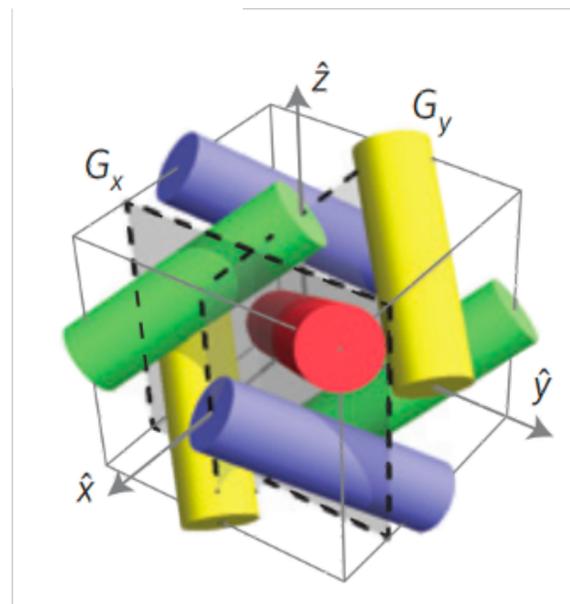
- Maxwell Equations (source free) satisfy Bloch's Theorem



$$\nabla \times (\nabla \times \mathbf{E}_{n\mathbf{k}}) = \omega_{n\mathbf{k}}^2 \mathbf{D}_{n\mathbf{k}}$$

$$\mathbf{D}_{n\mathbf{k}}(\mathbf{x}) = \epsilon(\mathbf{x})\mathbf{E}_{n\mathbf{k}}(\mathbf{x})$$

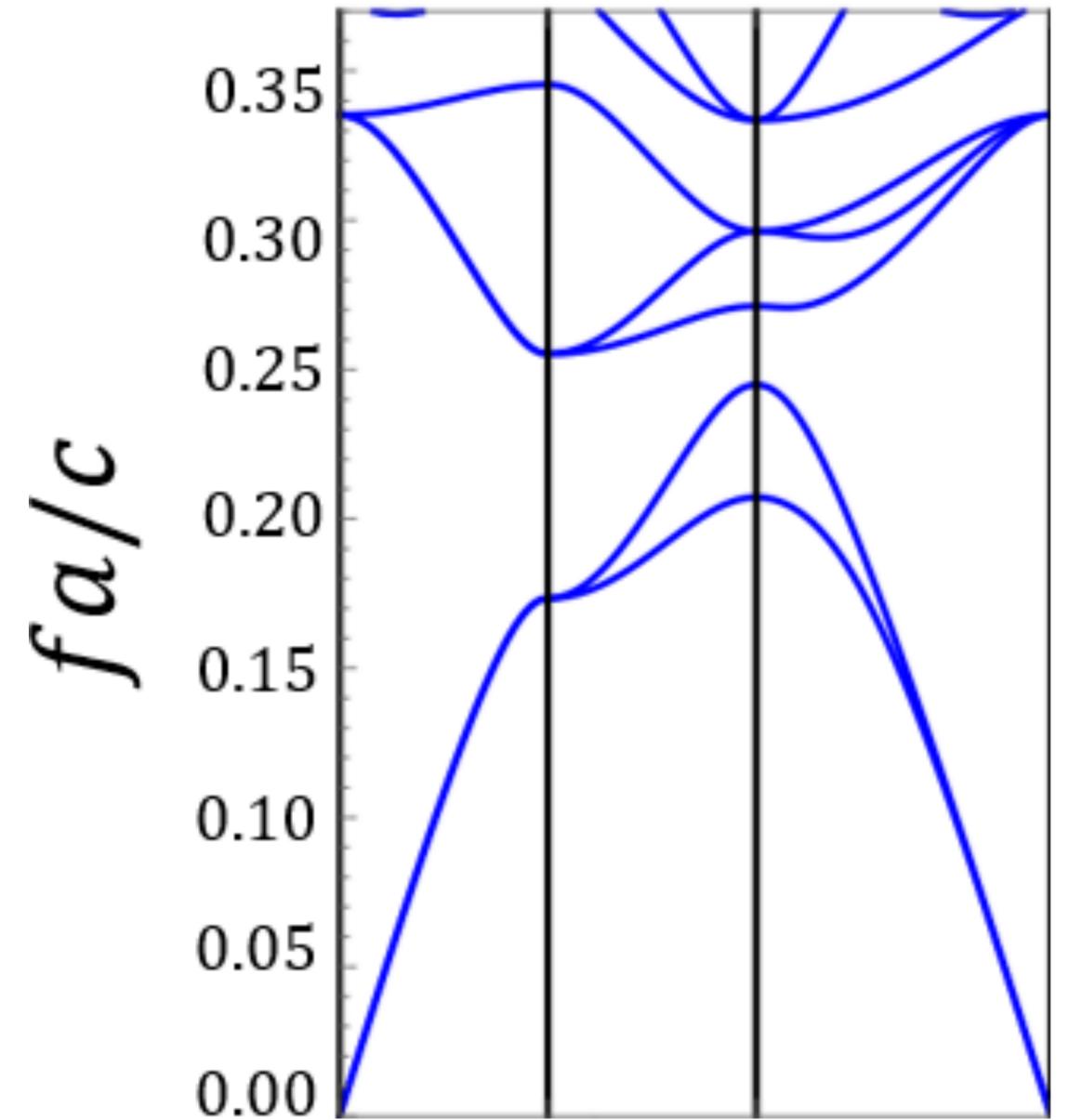
- Eigenfrequencies form bands



Lu et al, Nat Phys (2016)

Motivation: Modeling Topological Photonic Crystals

- **Gapped sets of bands can have nontrivial topology**
- **Need methods for computing topological invariants in the bulk**
- **Need models that capture topology without needing to solve Maxwell's equations for large finite systems**



Momentum Space: Wilson Loops and Symmetry Indicators

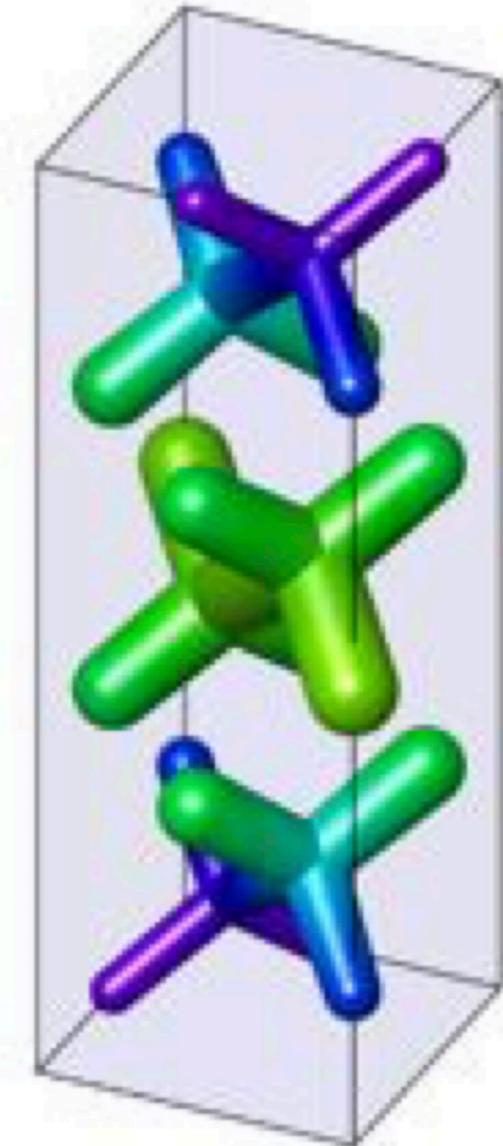
- General magnetoelectric material:

$$\begin{pmatrix} \mathbf{D}(t, \mathbf{r}) \\ \mathbf{B}(t, \mathbf{r}) \end{pmatrix} = \mathcal{K}(\mathbf{r}) \begin{pmatrix} \mathbf{E}(t, \mathbf{r}) \\ \mathbf{H}(t, \mathbf{r}) \end{pmatrix}$$

$$\mathcal{K}(\mathbf{r}) = \begin{pmatrix} \varepsilon(\mathbf{r}) & \xi(\mathbf{r}) \\ \xi^\dagger(\mathbf{r}) & \mu(\mathbf{r}) \end{pmatrix}$$

$$\mathcal{M}(\mathbf{k})u_{n,\mathbf{k}}(\mathbf{r}) = \omega_n(\mathbf{k})u_{n,\mathbf{k}}(\mathbf{r}),$$

$$\mathcal{M}(\mathbf{k}) = \mathcal{K}^{-1}\text{Rot}(\mathbf{k}) = \mathcal{K}^{-1} \begin{pmatrix} 0 & +(i\nabla_{\mathbf{r}} - \mathbf{k})\times \\ -(i\nabla_{\mathbf{r}} - \mathbf{k})\times & 0 \end{pmatrix}$$



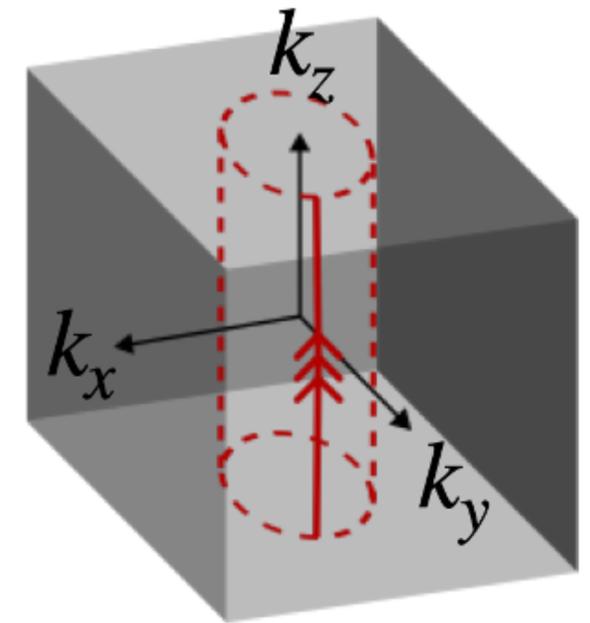
Momentum Space: Wilson Loops and Symmetry Indicators

- Topological invariants can be computed from Berry phases

$$\langle u|v\rangle_{\mathcal{K}} = \int_{\text{UC}} d^3\mathbf{r} u^\dagger(\mathbf{r})\mathcal{K}(\mathbf{r})v(\mathbf{r}),$$

$$\mathcal{W}_{m,n}^{\mathbf{k}+\boldsymbol{\epsilon}\leftarrow\mathbf{k}}(\boldsymbol{\epsilon}) = \langle u_{m,\mathbf{k}+\boldsymbol{\epsilon}}|u_{n,\mathbf{k}}\rangle_{\mathcal{K}},$$

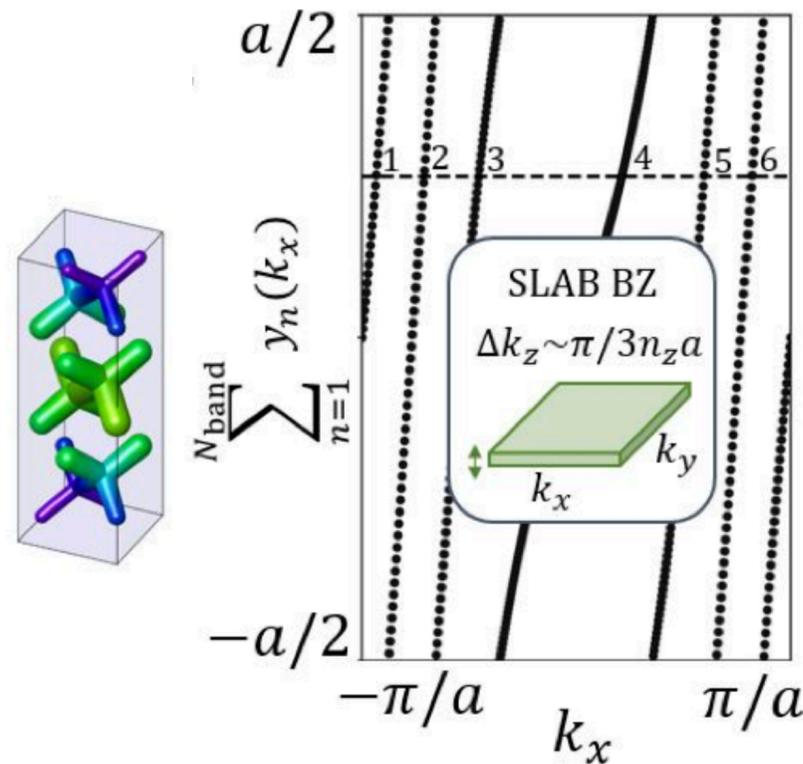
$$\mathcal{W}_{m,n}(\ell) = \mathcal{W}_{m,p}^{\mathbf{k}^{(F)}\leftarrow\mathbf{k}^{(N)}} \mathcal{W}_{p,q}^{\mathbf{k}^{(N)}\leftarrow\mathbf{k}^{(N-1)}} \dots \mathcal{W}_{r,s}^{\mathbf{k}^{(2)}\leftarrow\mathbf{k}^{(1)}} \mathcal{W}_{s,n}^{\mathbf{k}^{(1)}\leftarrow\mathbf{k}^{(0)}}$$



- Eigenvalues $e^{i w_n(\mathbf{k}_\perp)}$ related to projected position eigenvalues $\frac{w_n(\mathbf{k}_\perp)}{2\pi} = \frac{x_n(\mathbf{k}_\perp)}{a_x} \pmod{1}$,

Momentum Space: Wilson Loops and Symmetry Indicators

- Nontrivial topology appears in the winding of $w_n(\mathbf{k}_\perp)$

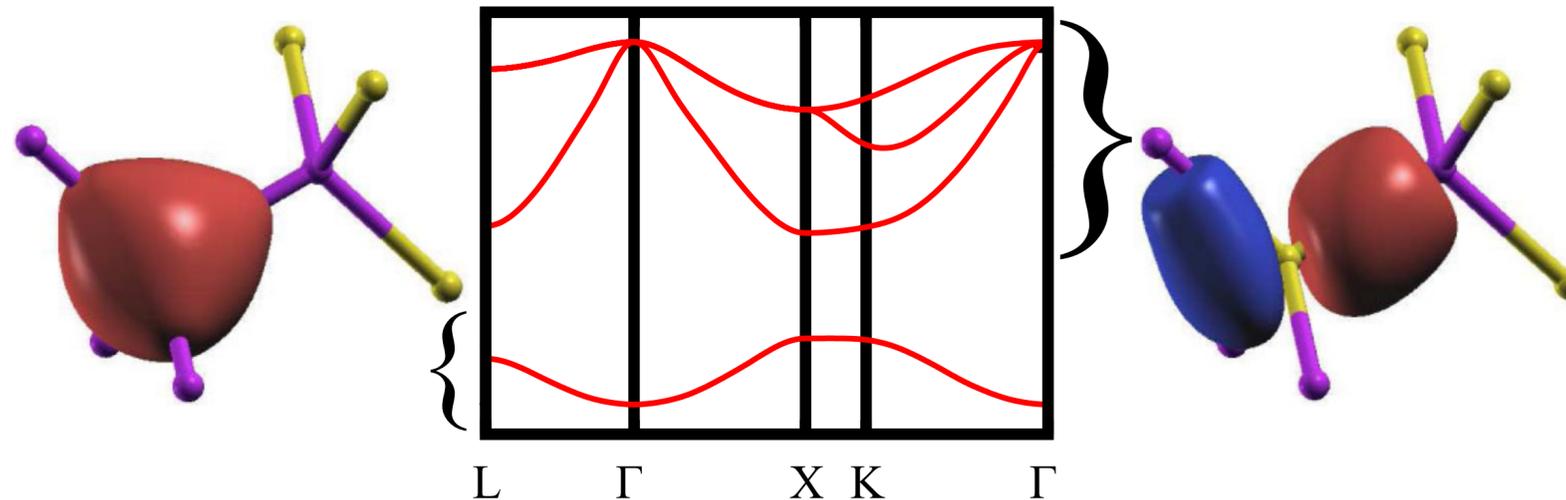


- Bulk-boundary correspondence: Winding of $w_n(\mathbf{k}_\perp)$ related to edge spectral flow**

- $\frac{w_n(\mathbf{k}_\perp)}{2\pi} = \frac{x_n(\mathbf{k}_\perp)}{a_x} \pmod{1}$, **implies a deep connection between topology and localization**

Momentum Space: Wilson Loops and Symmetry Indicators

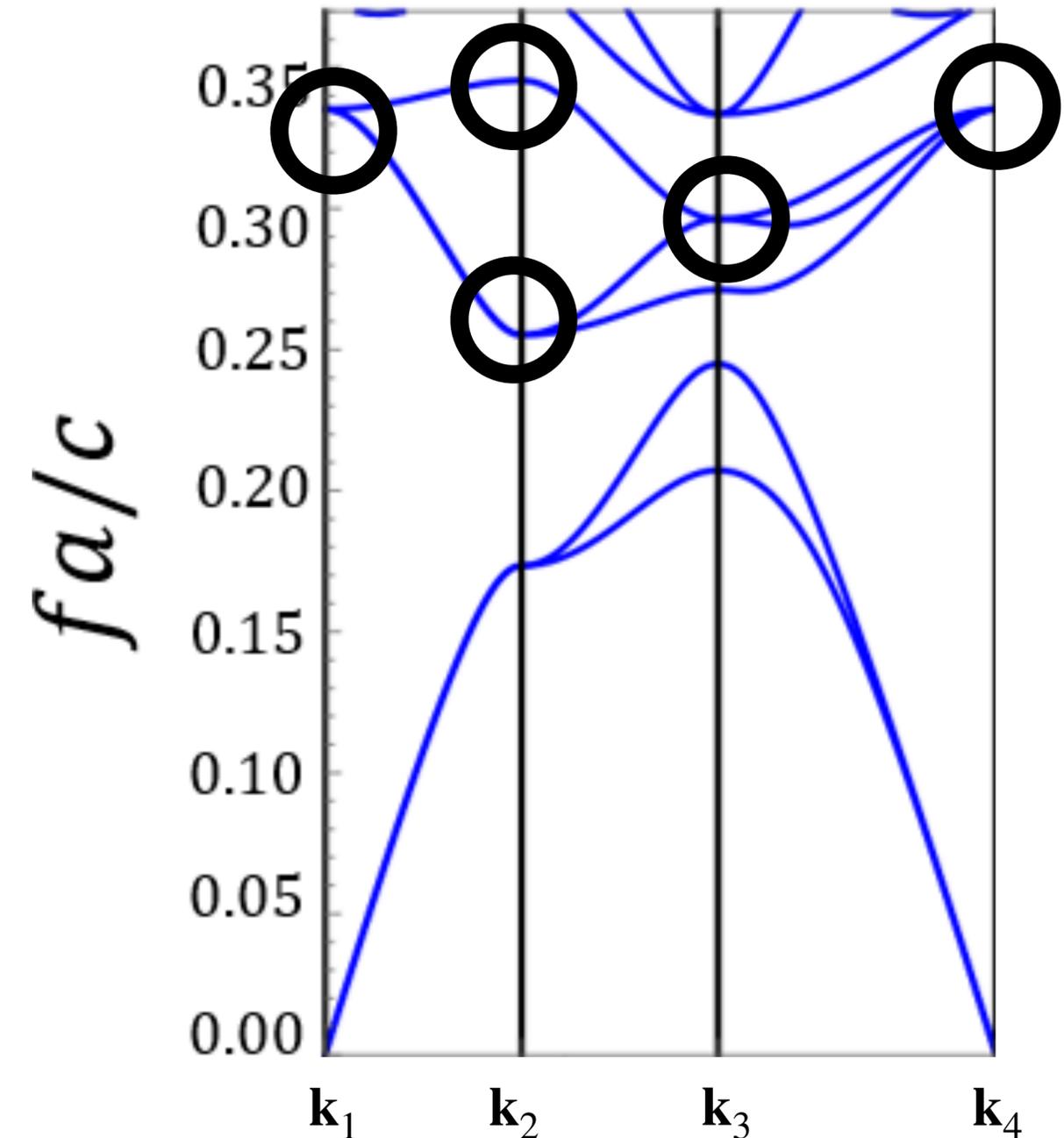
- **Topological invariants are obstructions to finding exponentially localized Wannier functions**



- **Wilson loop winding obstructs Fourier transform**
- **Space group symmetries let us define *symmetry indicators of band topology***

Momentum Space: Wilson Loops and Symmetry Indicators

- Eigenstates transform in irreps of the little group at each \mathbf{k}
- Collect irreps at high symmetry points into a symmetry data vector \mathbf{v}
- Topological Quantum Chemistry: for each space group, we can define a matrix Σ of symmetry indicators
- $\Sigma \mathbf{v} \neq 0$ implies nontrivial topology



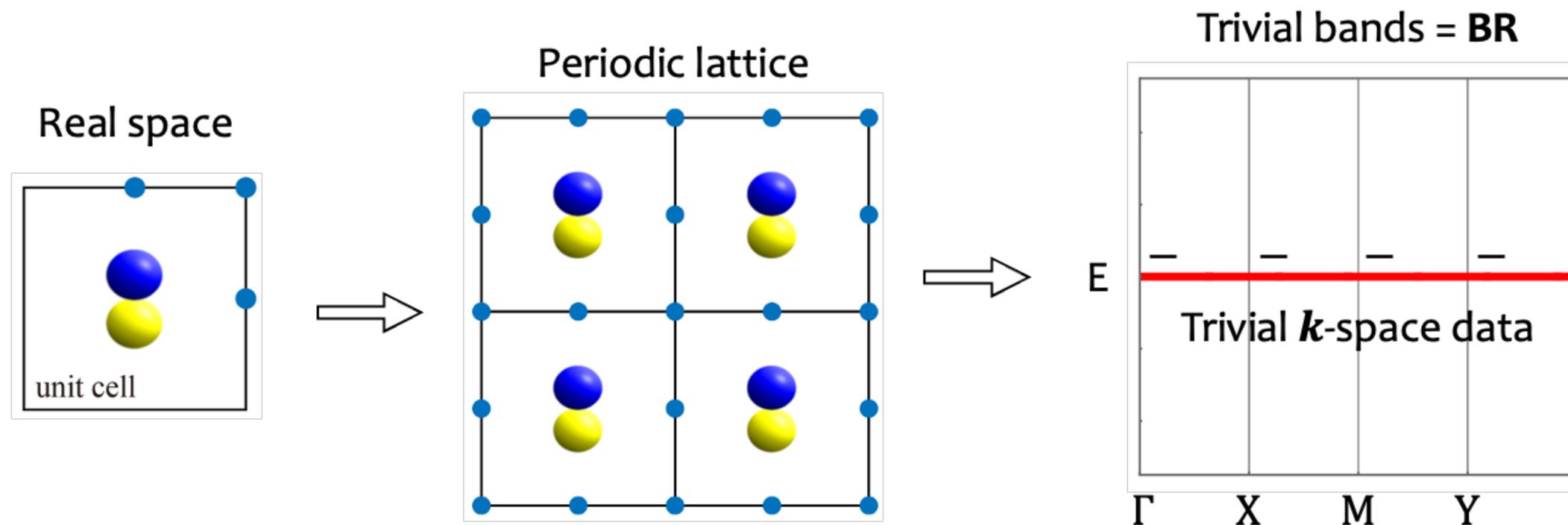
Challenges

- **General:**
 - **There exist topological invariants invisible to symmetry indicators**
 - **Symmetry indicators don't capture that different trivial phases may still be distinct**
- **Photonic specific: The lowest photonic bands are singular in 3D -> no well-defined symmetry data vector**

All have the same solution - Stable Real Space Invariants

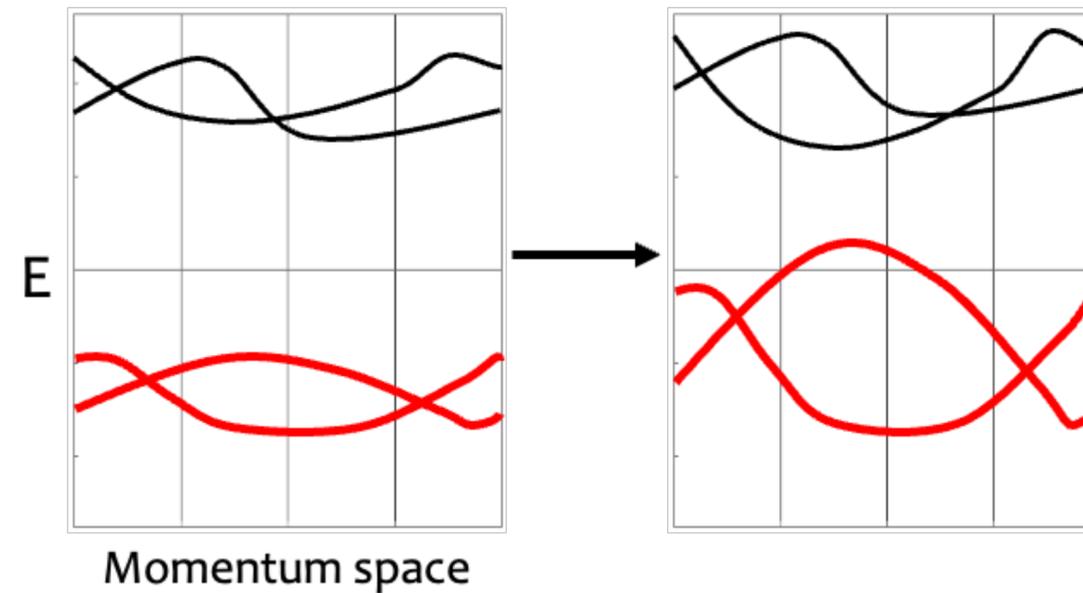
Wannier Functions and Band Representations

- End goal will be finite-rank modeling of photonic bands via tight-binding models -> need to understand *where* symmetry data vectors come from
- Topologically trivial bands have symmetric, localized Wannier functions by definition, determine symmetry data vectors by *induction*



Wannier Functions and Band Representations

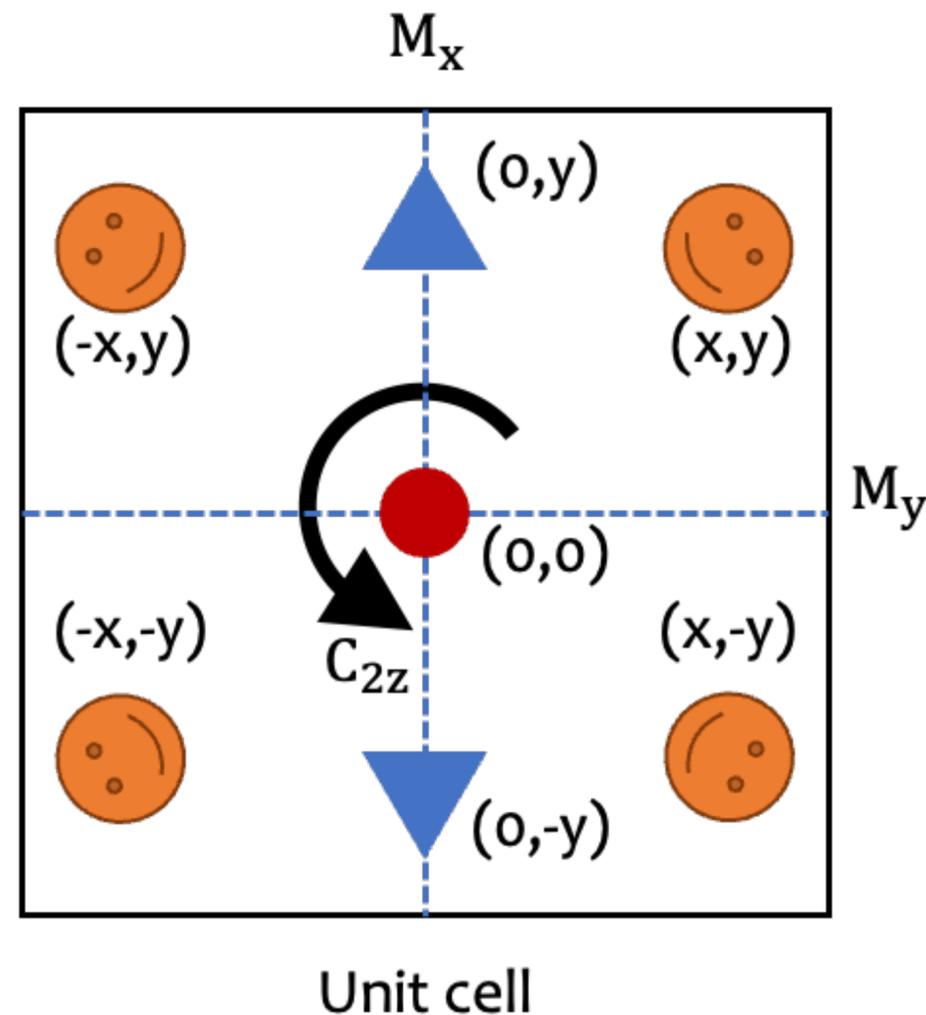
- **Band representations do not change under adiabatic deformation**



- **We can characterize trivial bands in terms of the symmetry properties and centers of the Wannier functions that induce them**

Wannier Functions and Band Representations

- Classify trivial bands by specifying location and symmetry properties of Wannier functions (orbitals) in the unit cell



Points in the unit cell fall into orbits called Wyckoff Positions (WP)

1. WP $1a(0,0)$ ●

At $(0,0)$: PG $mm2$

	1	C_{2z}	M_x	M_y
A_1	1	1	1	1
A_2	1	1	-1	-1
B_1	1	-1	-1	1
B_2	1	-1	1	-1

e.g. “ A_1 orbital” or “irrep”

2. WP $2g\{(0,y)+(0,-y)\}$ ▲

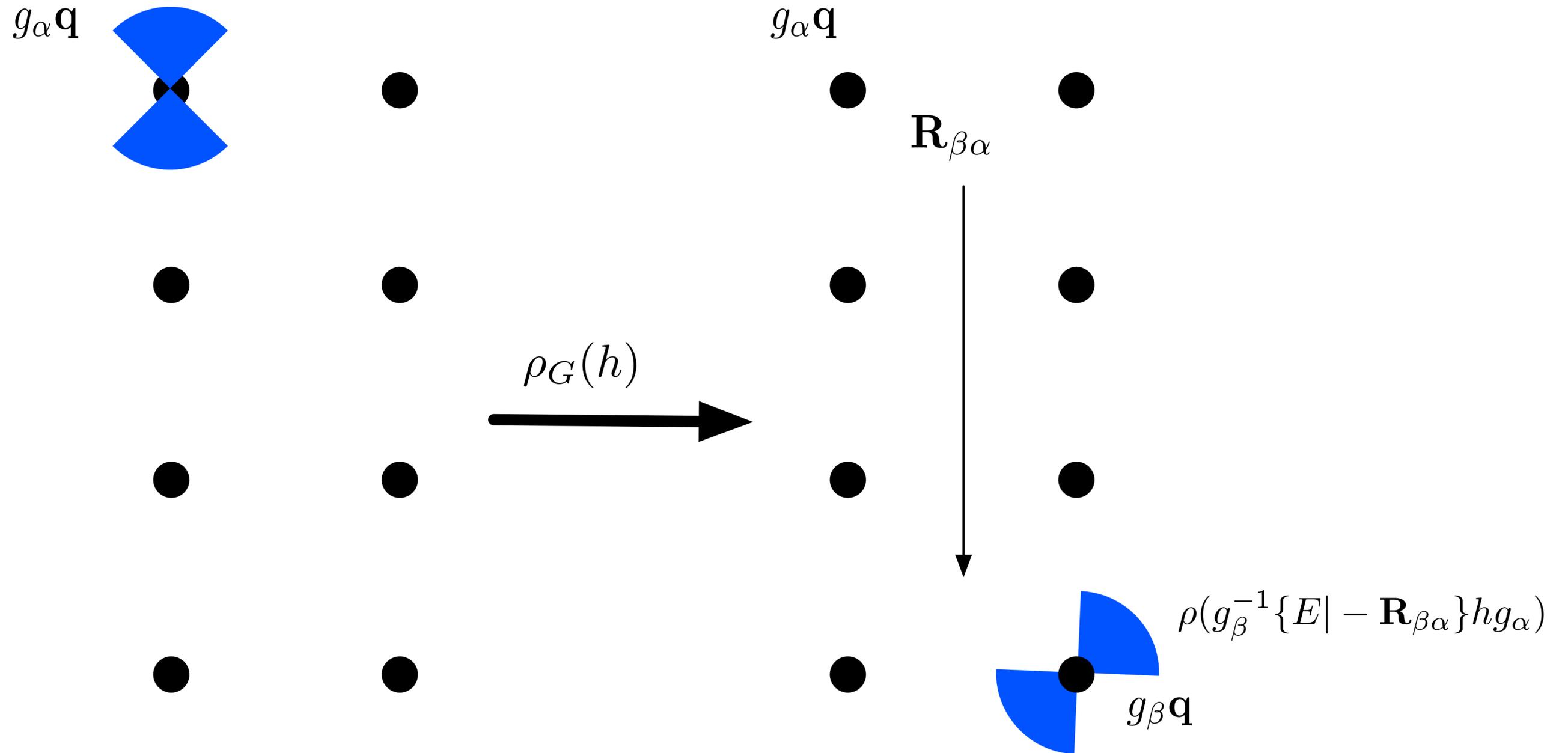
At $(0,y)$: PG m
Same at $(0,-y)$

3. WP $4i\{(x,y)+(-x,-y)+(-x,y)+(x,-y)\}$

At each position e.g. (x,y) : trivial PG

Only trivial A orbital

Wannier Functions and Band Representations

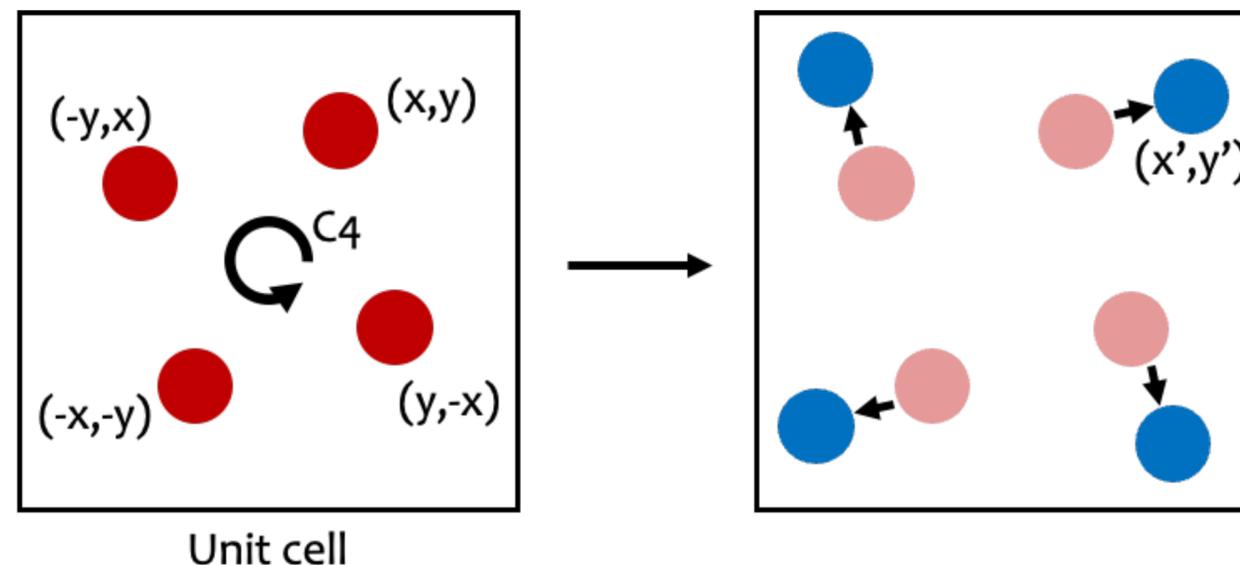


Wannier Functions and Topology

- Trivial band Wannier functions characterized by orbital multiplicity vector

$$\mathbf{m} = [m(\text{orb}_{1,\text{WP}_1}), m(\text{orb}_{2,\text{WP}_1}), \dots, m(\text{orb}_{M,\text{WP}_N})]^T$$

- Induction: $\mathbf{v} = B\mathbf{m}$. B is the *band representation matrix*
- Overcomplete: \mathbf{m} is not a topological invariant, can be changed by a choice of gauge. Corresponds to "moving" Wannier orbitals without breaking symmetry



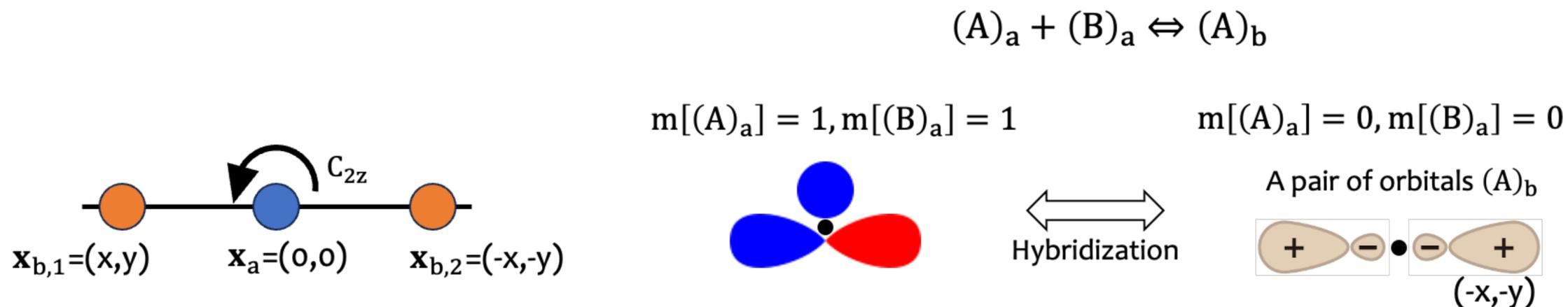
Wannier Functions and Topology

- Trivial band Wannier functions characterized by orbital multiplicity vector

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Adiabatic Processes

- For every space group, we can consider the collection of these “adiabatic processes” into a matrix q

- Columns of q : $(A)_a + (B)_a \Leftrightarrow (A)_b \rightarrow (1, 1, -1)$

- Can use Smith Decomposition to derive a set of adiabatic invariants:

$$q = L \cdot \Lambda \cdot R$$

$$\text{diag}(\Lambda) = (\lambda_1, \dots, \lambda_1, \lambda_2, \dots, \lambda_2, \dots, \lambda_M, \dots, \lambda_M, 0, \dots, 0)$$

- Since R and L are unimodular matrices, under any adiabatic process

$$(L^{-1} \cdot \Delta m)_i = \begin{cases} 0 \pmod{\Lambda_{ii}} & \text{for } i \leq \text{rank}(q) \\ 0 & \text{for } i > \text{rank}(q). \end{cases}$$

Stable Real Space Invariants - Construction

- This means that L^{-1} defines a set of invariants that do not change under any adiabatic process

$$\begin{aligned}\tilde{\Theta}^{(\lambda_1)} &= (L^{-1})_{1, \dots, n_{\lambda_1}, *} \pmod{\lambda_1}, \\ \tilde{\Theta}^{(\lambda_2)} &= (L^{-1})_{n_{\lambda_1}+1, \dots, n_{\lambda_1}+n_{\lambda_2}, *} \pmod{\lambda_2}, \quad \dots \\ \tilde{\Theta}^{(\lambda_M)} &= (L^{-1})_{n_{\lambda_1}+\dots+n_{\lambda_{M-1}}+1, \dots, N_{UC}^\rho-n_0, *} \pmod{\lambda_M}, \\ \tilde{\Theta}^{(0)} &= (L^{-1})_{N_{UC}^\rho-n_0+1, \dots, N_{UC}^\rho, *},\end{aligned}$$

- These are the stable real space invariants (stable RSIs). Tabulated for all space groups

Stable Real Space Invariants - Meaning

- **Theorem: Two sets of trivial bands \mathbf{m}_1 and \mathbf{m}_2 have the same stable RSIs, i.e.**

$$(\mathbf{L}^{-1} \cdot (\mathbf{m}_1 - \mathbf{m}_2))_i = \begin{cases} 0 \pmod{\Lambda_{ii}} & \text{for } i \leq \text{rank}(q) \\ 0 & \text{for } i > \text{rank}(q). \end{cases}$$

if and only if there exists some auxiliary trivial bands \mathbf{m}_{aux} such that $\mathbf{m}_1 + \mathbf{m}_{\text{aux}}$ and $\mathbf{m}_2 + \mathbf{m}_{\text{aux}}$ can be adiabatically deformed into each other \rightarrow stable equivalence

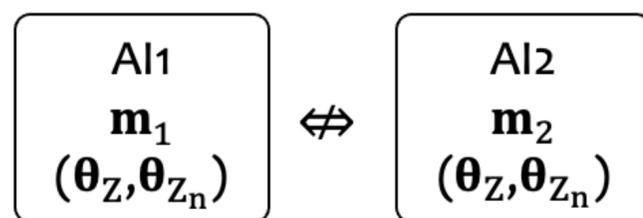
Stable Real Space Invariants - Meaning

- Theorem: Two sets of trivial bands \mathbf{m}_1 and \mathbf{m}_2 have the same stable RSIs, i.e.**

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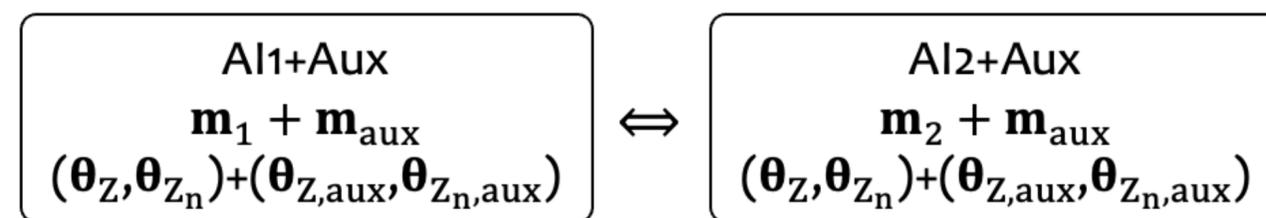
if and only if there exists some auxiliary trivial bands \mathbf{m}_{aux} such that $\mathbf{m}_1 + \mathbf{m}_{\text{aux}}$ and $\mathbf{m}_2 + \mathbf{m}_{\text{aux}}$ can be adiabatically deformed into each other \rightarrow stable equivalence

Two phases Al1 and Al2 may not be deformable (topologically distinct)



*BR multiplicity \mathbf{m} determines stable RSIs (θ_z, θ_{z_n}) [many-to-one]

$(\text{Al1} + \text{Aux})$ and $(\text{Al2} + \text{Aux})$ are equivalent for certain additional orbitals (trivial bands) Aux



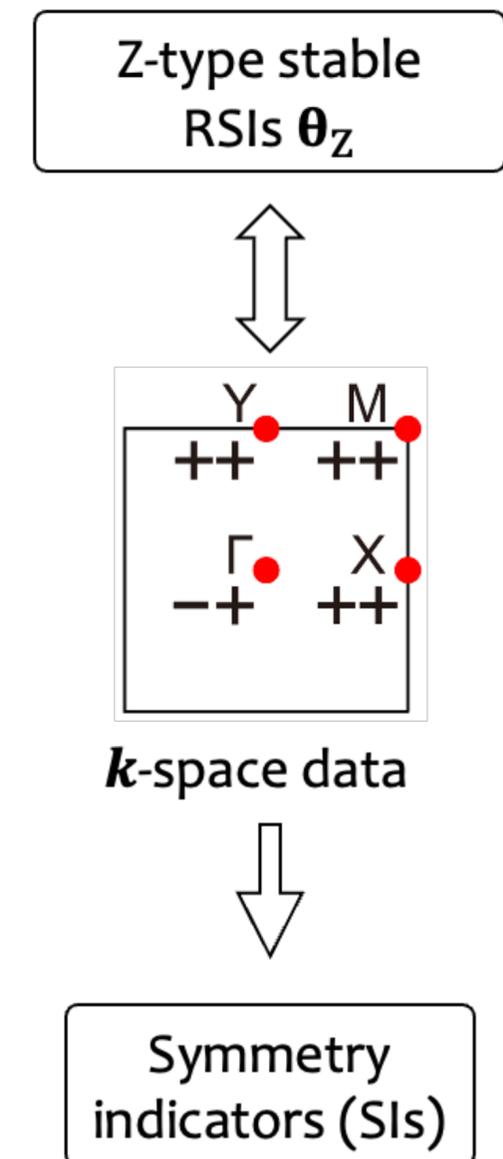
Deformable with extra orbitals!

Stable Real Space Invariants - Meaning

- Integer valued stable RSIs uniquely determine the symmetry data vector, and vice versa: $\mathbf{v} = \mathcal{M}\theta_{\mathbb{Z}}$
- mod n stable RSIs contain info beyond momentum space data

Stable Real Space Invariants - Meaning

- Integer valued stable RSIs uniquely determine the symmetry data vector, and vice versa: $\mathbf{v} = \mathcal{M}\theta_Z$
- mod n stable RSIs contain info beyond momentum space data



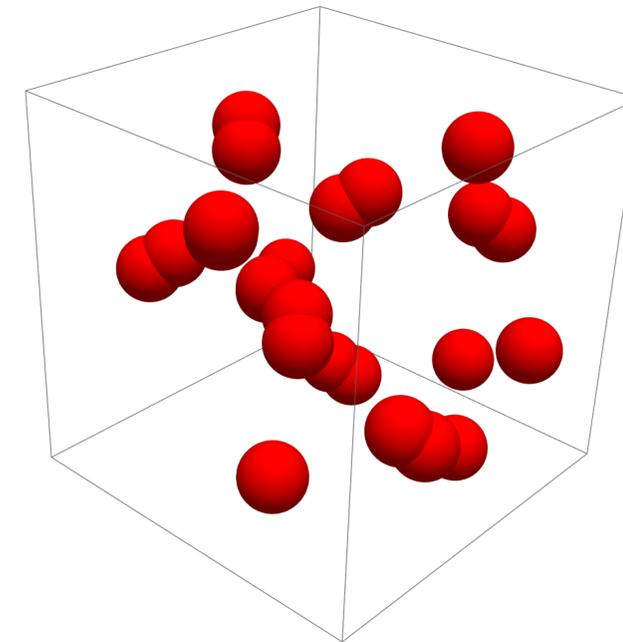
Atomic insulator (AI)
 \mathbf{m}_{AI} : well-defined BR/orbital
 k -space data : Well-defined
 (θ_Z, θ_{Z_n}) : Integer valued (Z or Zn)
 Zero SI

Topological insulator (TI)
 \mathbf{m}_{TI} : NOT defined (by definition)
 k -space data : Still well-defined
 θ_Z : Determined from k -space data
 Fractional $\theta_Z \Leftrightarrow$ Nonzero SI

Example: Space Group 212

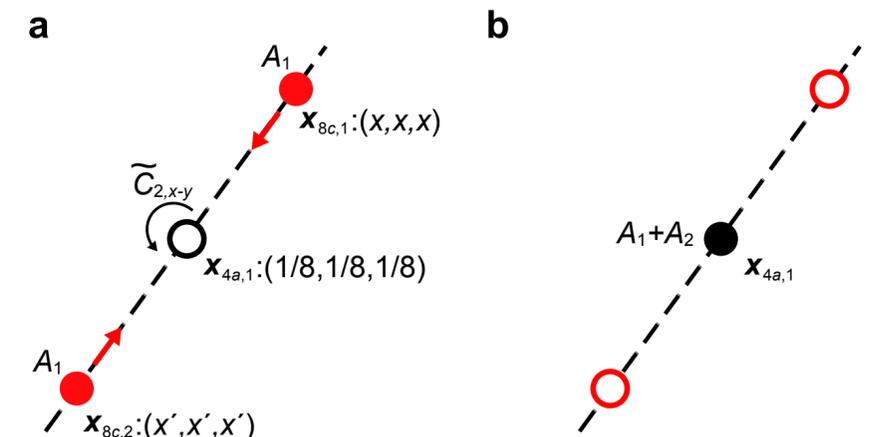
- Generators: Cubic 3fold rotation, fourfold screw rotation, twofold screw rotation

WP W	G_W	$(\rho)_W$
$4a(1/8, 1/8, 1/8)$	$C_{3,111}, \tilde{C}_{2,x-y}$	$(A_1)_a, (A_2)_a, (E)_a$
$4b(5/8, 5/8, 5/8)$	$C_{3,111}, \tilde{C}'_{2,x-y}$	$(A_1)_b, (A_2)_b, (E)_b$
$8c(x, x, x)$	$C_{3,111}$	$(A_1)_c, ({}^1E^2E)_c$
$12d(y, 1/4 - y, 1/8)$	$\tilde{C}_{2,x-y}$	$(A)_d, (B)_d$
$24e(x, y, z)$	$\{E \mathbf{0}\}$	$(A)_e$



- Adiabatic processes

$$\begin{aligned}
 (A_1 + A_2)_a &\Leftrightarrow (A_1)_c, & 2(E)_a &\Leftrightarrow ({}^1E^2E)_c, \\
 (A_1 + A_2)_b &\Leftrightarrow (A_1)_c, & 2(E)_b &\Leftrightarrow ({}^1E^2E)_c, \\
 (A_1 + E)_a &\Leftrightarrow (A)_d, & (A_2 + E)_a &\Leftrightarrow (B)_d, \\
 (A_1 + E)_b &\Leftrightarrow (A)_d, & (A_2 + E)_b &\Leftrightarrow (B)_d, \\
 (A + {}^1E^2E)_c &\Leftrightarrow (A)_e, & (A + B)_d &\Leftrightarrow (A)_e,
 \end{aligned}$$



Example: Space Group 212

$$q_{\text{adia}} = \begin{pmatrix} 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 2 & 1 & 1 & 0 & 0 \\ -1 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 & 0 & 1 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & -1 \end{pmatrix} \begin{matrix} (A_1)_a \\ (A_2)_a \\ (E)_a \\ (A_1)_b \\ (A_2)_b \\ (E)_b \\ (A_1)_c \\ ({}^1E^2E)_c \\ (A)_d \\ (B)_d \\ (A)_e \end{matrix}$$

Example: Space Group 212

$$L = \begin{pmatrix} 1 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 2 & 1 & 1 & 0 & -2 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 1 & 1 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 3 & 1 & -2 & -1 & -1 & 1 \\ -1 & 0 & 0 & 0 & -1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & -1 & -1 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

$$\text{diag } \Lambda = (1, 1, 1, 1, 1, 1, 1, 1, 2, 0, 0),$$

$$R = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 1 & 0 & 0 & 0 & 1 & 0 & -1 \\ 0 & 0 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & -2 & 1 & -3 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & -1 & 0 & -1 & 0 & 1 \end{pmatrix}.$$

Example: Space Group 212

$$(L^{-1})_{8,*} \pmod{2} = (1, 1, 1, 0, 0, \dots, 0),$$

$$\begin{pmatrix} (L^{-1})_{9,*} \\ (L^{-1})_{10,*} \\ (L^{-1})_{11,*} \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 1 & 0 & 1 & 0 & 0 & 1 & 1 \\ 0 & 0 & 1 & 0 & 0 & 1 & 0 & 2 & 1 & 1 & 2 \end{pmatrix}.$$

- **Three integer invariants, and one mod 2 invariant**

$$\theta_1 = m[(A_1)_a] + m[(A_1)_b] + m[(A_1)_c] \\ + m[(A)_d] + m[(A)_e],$$

$$\theta_2 = m[(A_2)_a] + m[(A_2)_b] + m[(A_1)_c] \\ + m[(B)_d] + m[(A)_e],$$

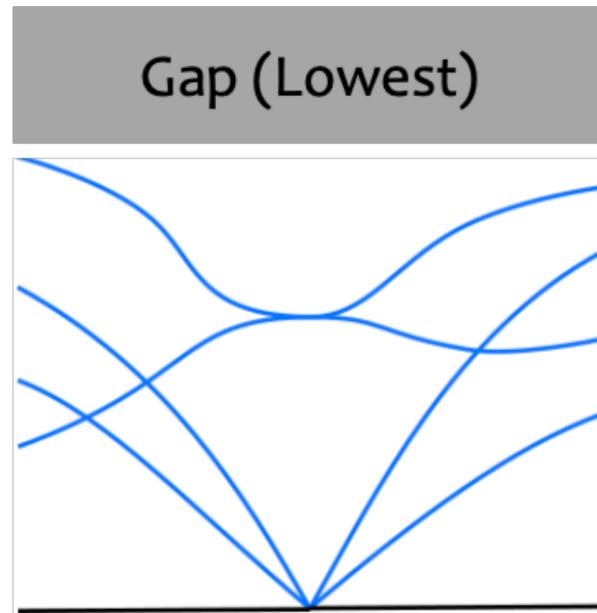
$$\theta_3 = m[(E)_a] + m[(E)_b] + 2m[({}^1E^2E)_c] \\ + m[(A)_d] + m[(B)_d] + 2m[(A)_e],$$

$$\theta_4^{(2)} = m[(A_1)_a] + m[(A_2)_a] + m[(E)_a] \pmod{2}.$$

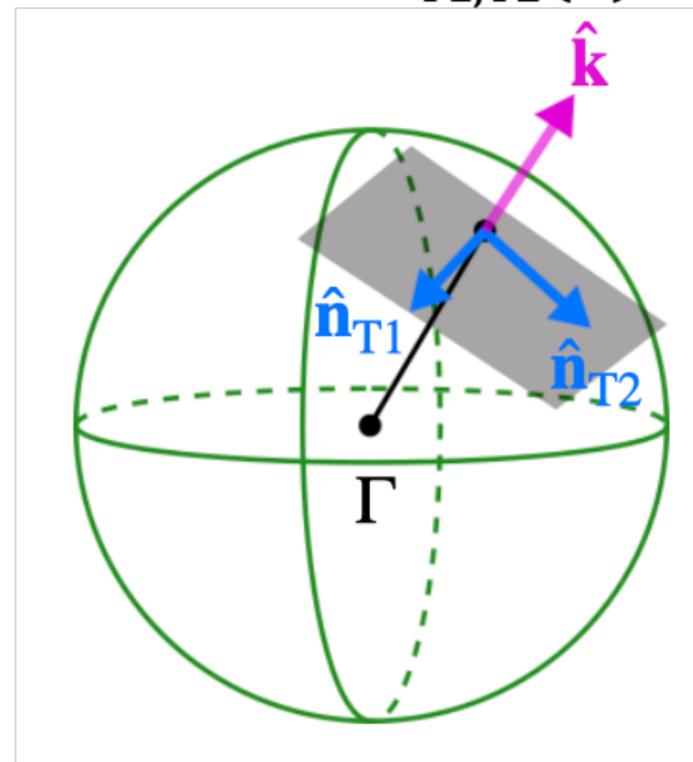
Photonics- The Lowest Bands

- The lowest photonic bands are pathological

Two transverse (T) modes
w/ linear dispersion



Transverse polarization
vectors $\hat{\mathbf{n}}_{T1,T2}(\mathbf{k})$



$$\mathbf{D}_{\mathbf{k}}^{T1}(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}}\hat{\mathbf{n}}_{T1} \quad \mathbf{D}_{\mathbf{k}}^{T2}(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}}\hat{\mathbf{n}}_{T2}$$

2T modes

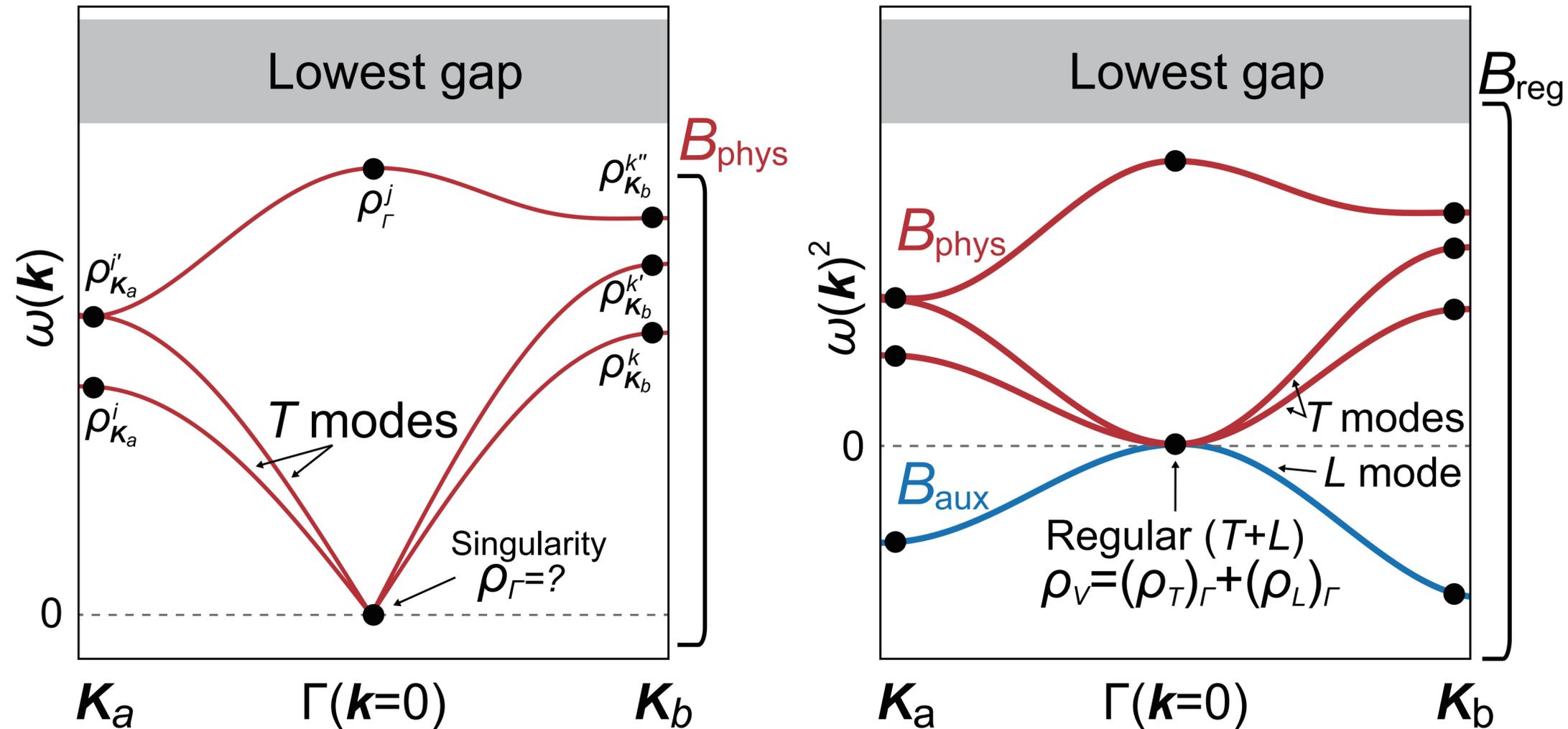
$$\mathbf{D}_{\mathbf{k}}^L(\mathbf{r}) \sim e^{i\mathbf{k}\cdot\mathbf{r}}\hat{\mathbf{k}}$$

1L mode

L mode forbidden by
transversality constraint
 $\nabla \cdot \mathbf{D} = 0$ i.e. $\mathbf{k} \cdot \mathbf{D}_{\mathbf{n}\mathbf{k}} = 0$

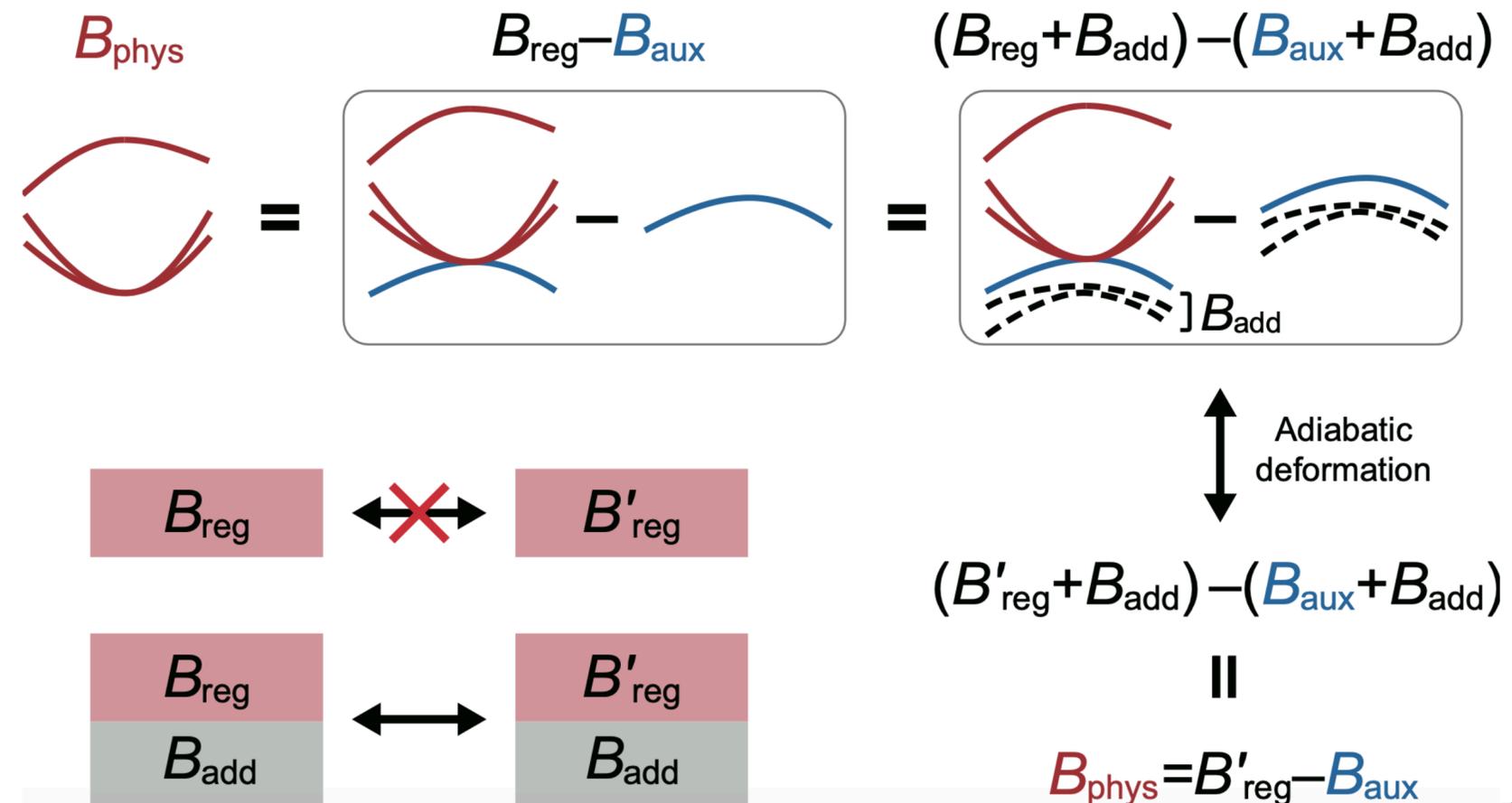
Photonics- The Lowest Bands

- We can cure the pathology by adding back in fictitious longitudinal bands as a mathematical trick, as long as we can subtract them later



Stable Equivalence and Photonic Bands

- Useful for modeling - can algorithmically search for the minimal auxiliary bands needed for a faithful tight binding model
- But what about classification? If we add even more auxiliary bands, nothing should change about the physics



Stable Equivalence and Photonic Bands

- **This means photonic bands are classified by stable equivalence classes of pairs $(\mathcal{B}_{\text{reg}}, \mathcal{B}_{\text{aux}})$**
- **These are classified by stable real space invariants!**
- **Transversality constraint: inequalities on the invariants that must be satisfied for any topologically trivial photonic band structure**

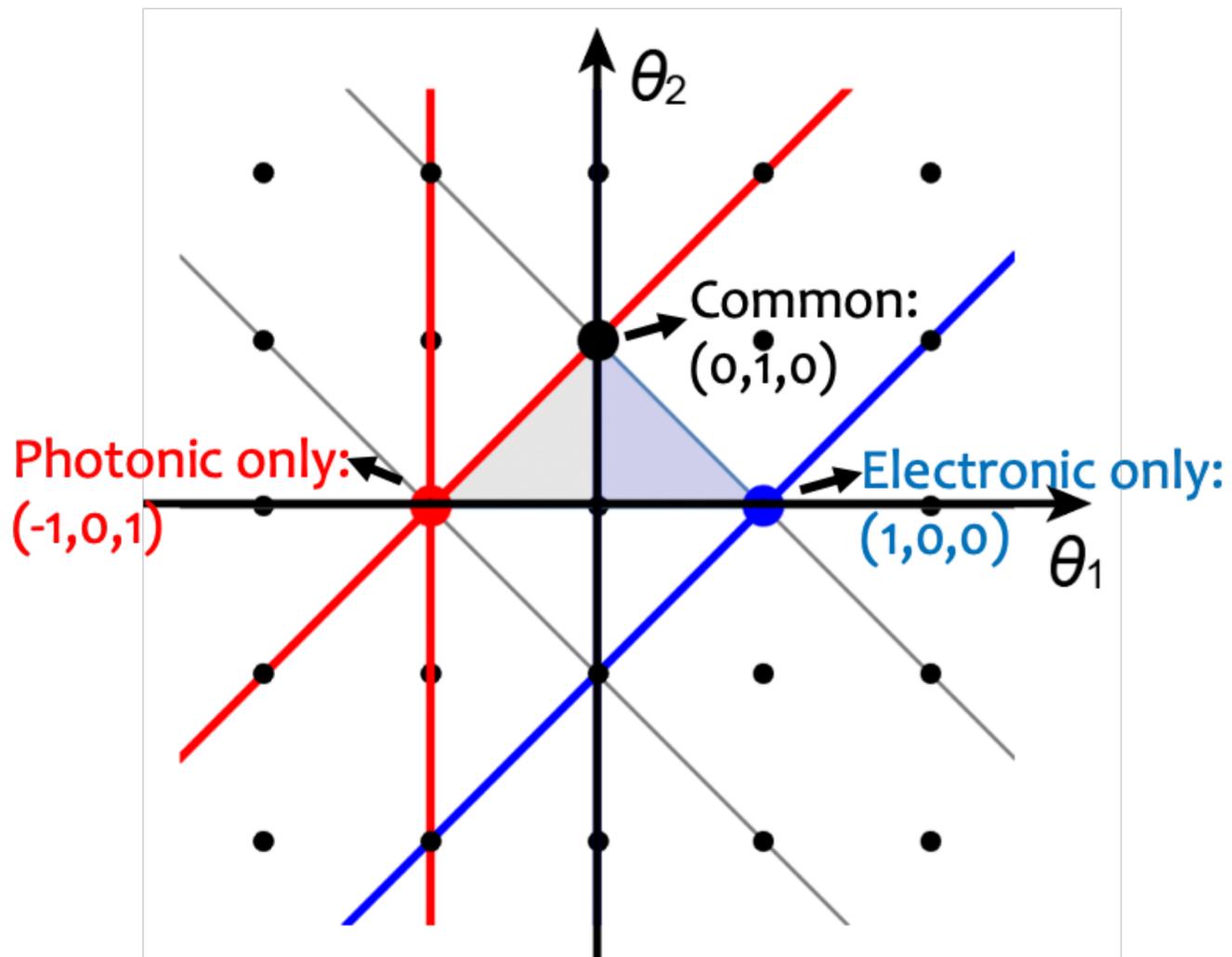
$$\mathcal{M}\theta_{\mathbb{Z}} \geq \mathbf{b}_{\text{ph}}$$

- **Can be solved via linear programming**

Stable Equivalence and Photonic Bands

- **Key point: This allows us to isolate “interesting” topology of the lowest band from the Euler characteristic of the polarization vector**
- **$\mathbf{b}_{\text{ph}} \neq \mathbf{b}_{\text{electron}}$ implies photonic systems can realize trivial band structures that cannot appear in condensed matter**
- **Allows us to model band structures in a way that captures topological properties of Wilson loops**

Example: Space Group 212



Photonic bands [
 $(\blacksquare)_T = \Gamma_4 - \Gamma_1$]

$\theta_{\mathbf{z}}=(0,1,0)$: $((\blacksquare)_T + \Gamma_1 + \Gamma_2, R_3, M_2M_3 + M_5, X_1 + X_2)$

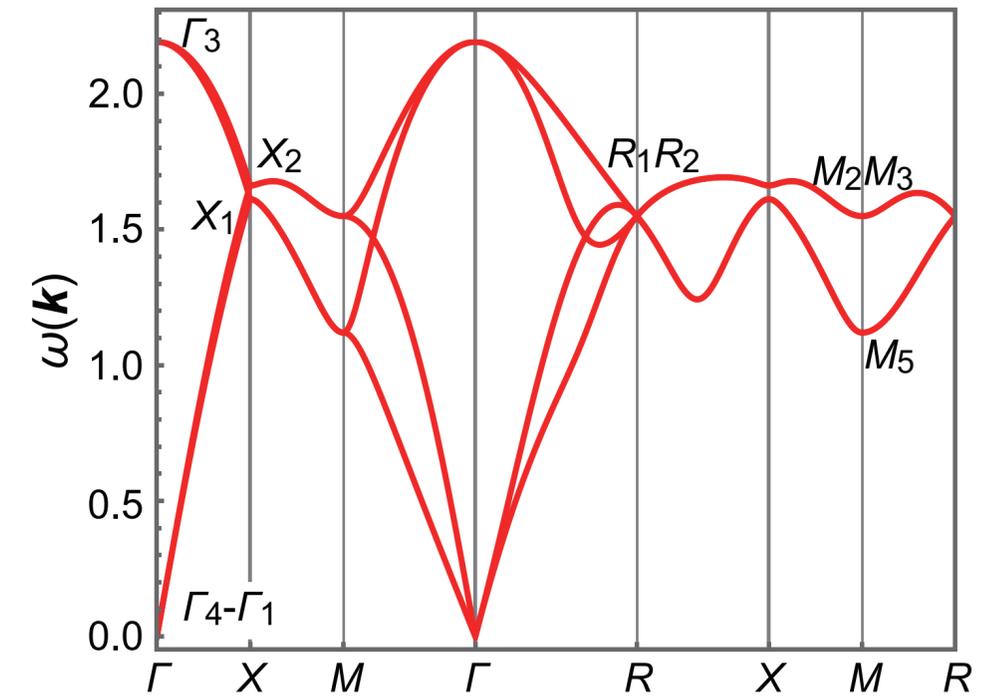
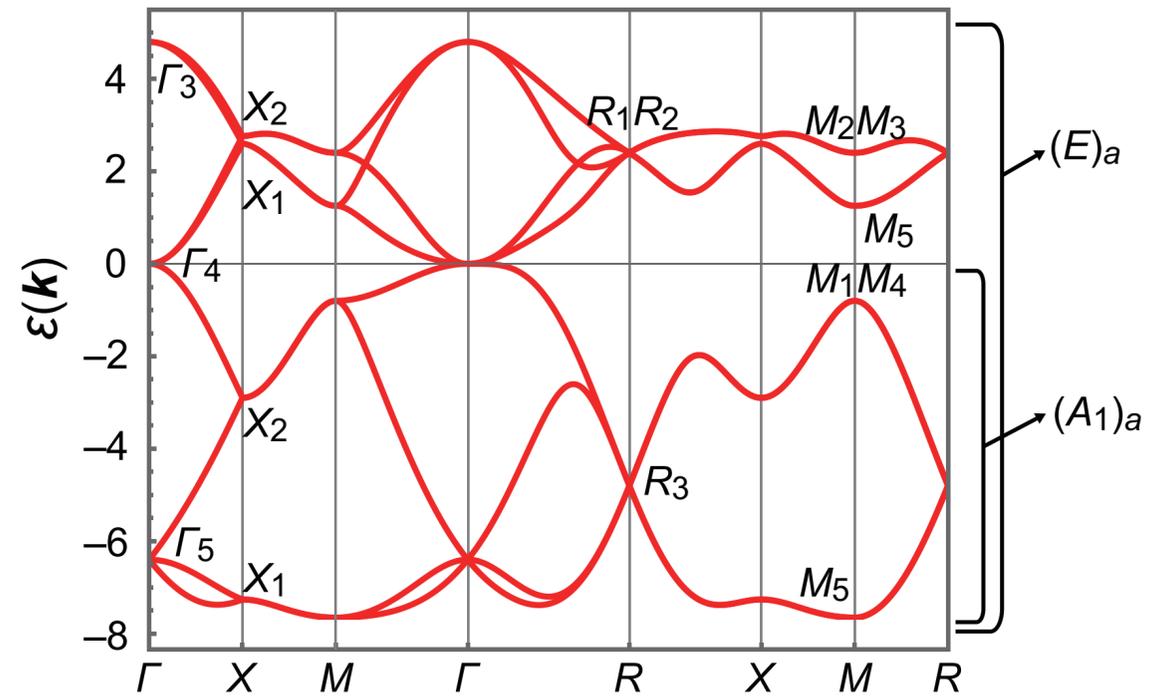
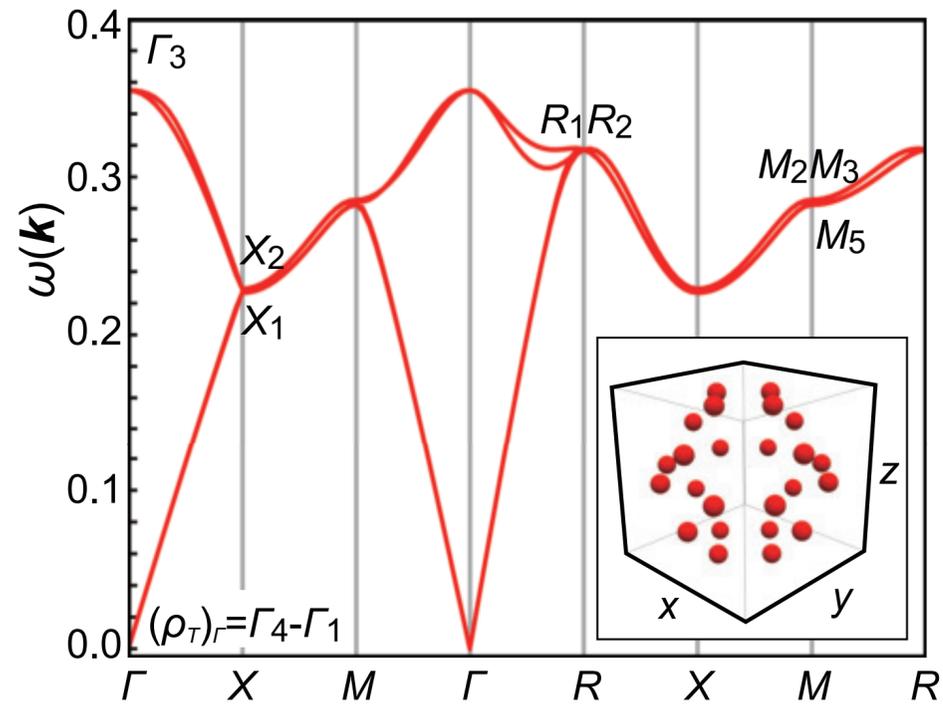
$\theta_{\mathbf{z}}=(-1,0,1)$: $((\blacksquare)_T + \Gamma_3, R_1R_2, M_2M_3 + M_5, X_1 + X_2)$,

Electronic bands

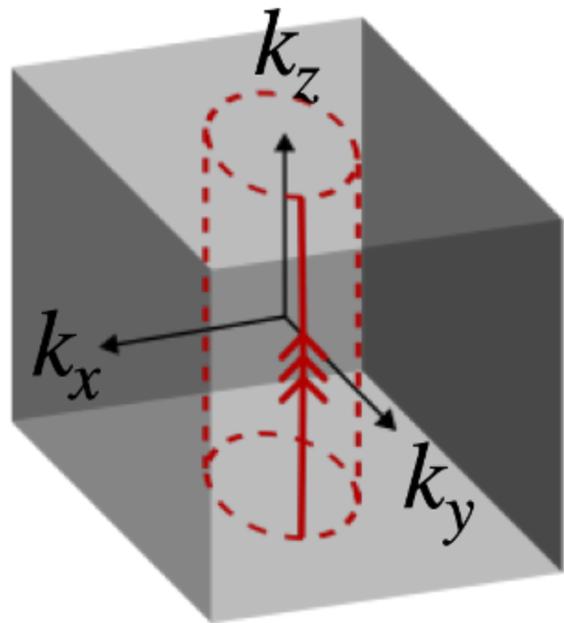
$\theta_{\mathbf{z}}=(0,1,0)$: $(\Gamma_2 + \Gamma_4, R_3, M_2M_3 + M_5, X_1 + X_2)$

$\theta_{\mathbf{z}}=(1,0,0)$: $(\Gamma_1 + \Gamma_5, R_3, M_1M_4 + M_5, X_1 + X_2)$

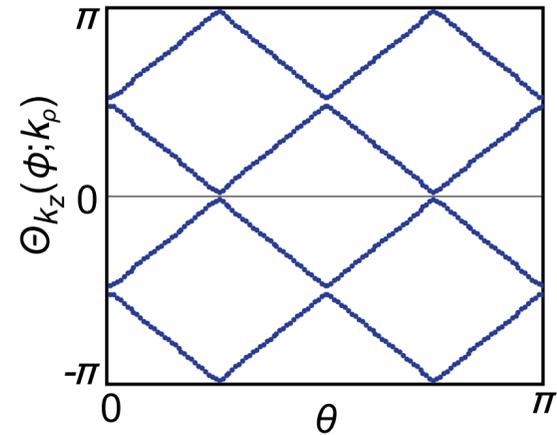
Example: Space Group 212



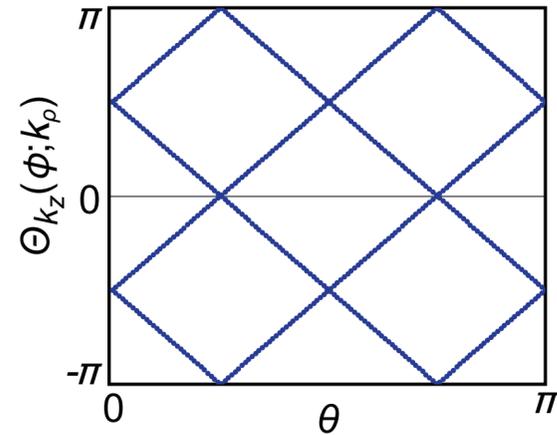
Example: Space Group 212



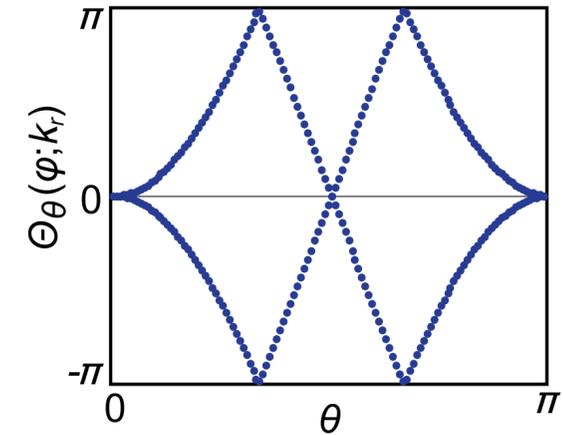
Cylindrical Wilson loop ($k_\rho=0.4\pi$)



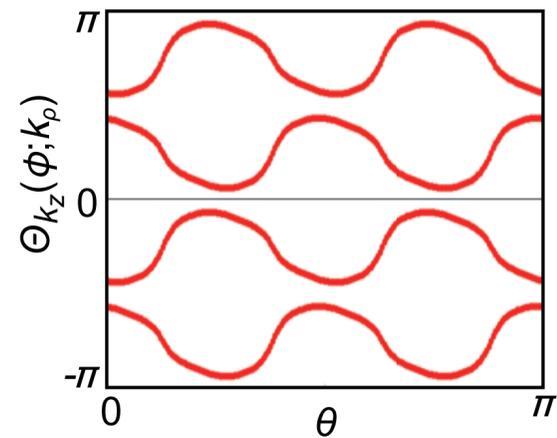
Cylindrical Wilson loop ($k_\rho=0.1\pi$)



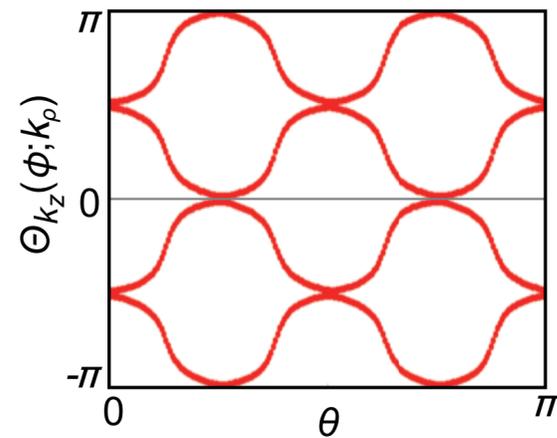
Spherical Wilson loop ($k_r=0.2\pi$)



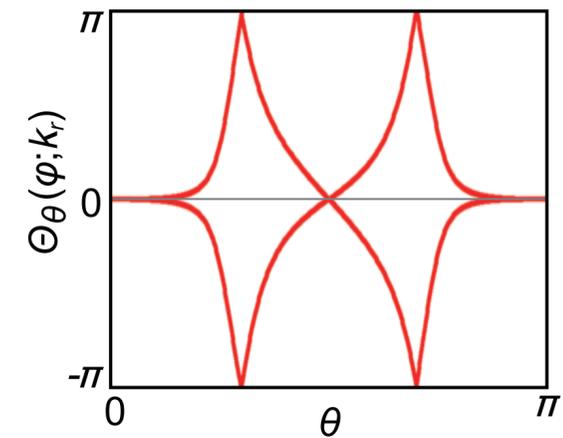
Cylindrical Wilson loop ($k_\rho=0.4\pi$)



Cylindrical Wilson loop ($k_\rho=0.1\pi$)



Spherical Wilson loop ($k_r=0.2\pi$)



Conclusion

- **Stable real space invariants characterize band topology beyond symmetry indicators**
- **They also give the natural classification of topologically trivial photonic bands**
- **Complete the extension of the theory of topological quantum chemistry to photonics**
- **References:**

Devescovi et al., Optical Materials Express 14, 2161-2177 (2024).

Hwang et al., to appear 2025 (x2)