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Multi-gap topology & non-abelian braiding in **k**-space

Gunnar F. Lange (GFL25@CAM.AC.UK)

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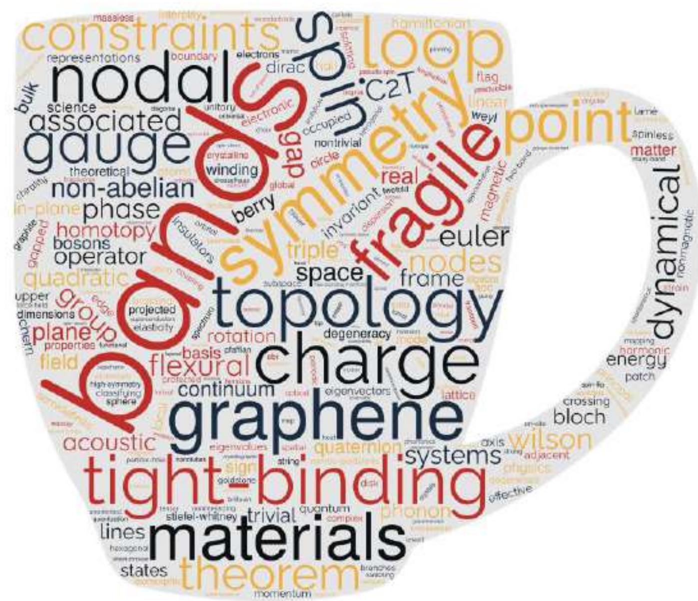
Outline

GFL25@CAM.AC.UK

- General comments on topology
- Homotopy theory
  - Generalities
  - Anyons
  - Band structures
- Weyl points
- Multi-gap topology
  - Formality
  - Applications
- Conclusion & Outlook

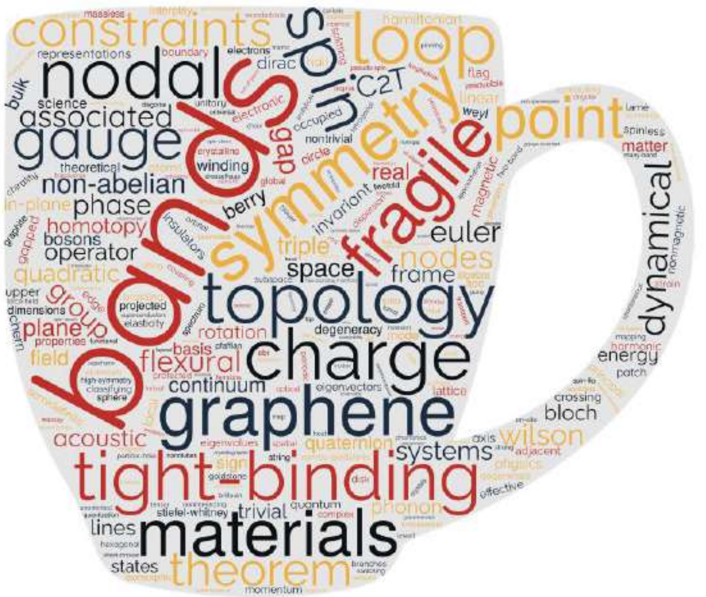


Topology?

- Study *global* properties of theories

- Robust experimental quantities

- Method today: Homotopy theory



Homotopy theory

- Study *mappings of paths*

$$S^N \to M$$

N-dimensional Sphere

Target manifold

Homotopy theory

- Study *mappings of paths*

$$S^N \to M$$

N-dimensional Sphere

Target manifold

- N-th homotopy group: $\pi_N(M)$

Homotopy theory

- Study *mappings of paths*

$$S^N \to M$$

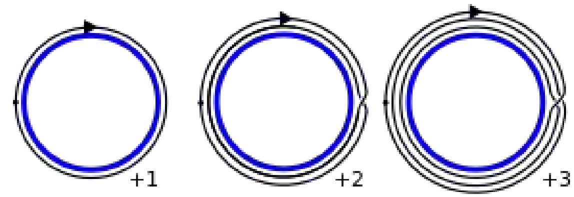
N-dimensional Sphere

Target manifold

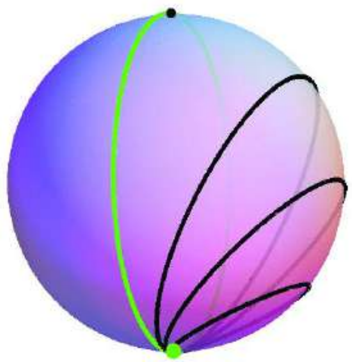
- N-th homotopy group: $\pi_N(M)$
  - Natural group structure: Composition of paths
  - Efficient algorithms exist to compute these groups

Homotopy examples

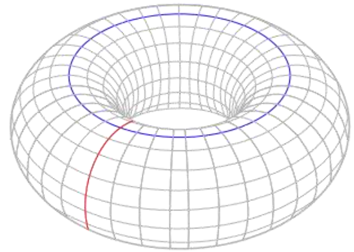
$$\pi_1(S^1) = \mathbb{Z}$$



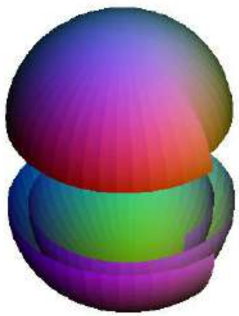
$$\pi_1(S^2) = \mathbb{0}$$



$$\pi_1(T^2) = \mathbb{Z} \times \mathbb{Z}$$



$$\pi_2(S^2) = \mathbb{Z}$$



Homotopy in physics

- Identical particles: Configuration space

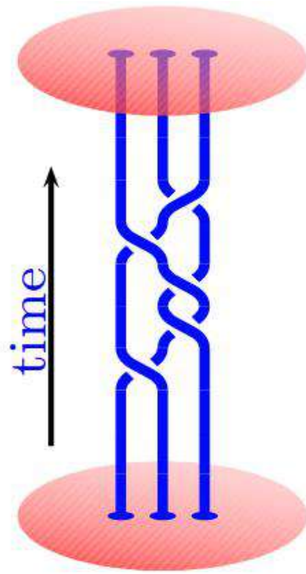
Particle number

Avoid overlapping particles

$$M_d^N = \frac{(\mathbb{R}^d)^N - \Delta}{S_N}$$

Spatial dimension

Divide by permutations of coordinates



S. Simon Topological Quantum: Lecture Notes (2021)

$$\pi_1(M_2^N) = B_N$$ ← Braid group

$$\pi_1(M_3^N) = S_N$$ ← Symmetric group

Homotopy in physics

$$\pi_1(M_2^N) = B_N$$ ← Braid group

- Abelian representations:
  - Anyons

- Non-abelian representations: ← Quantum computing
  - Non-abelian anyons

$$\pi_1(M_3^N) = S_N$$ ← Symmetric group

- Abelian representations:
  - Boson/Fermions

- Non-abelian representations: ← Not too relevant for point particles
  - Parastatistics

Central question

Can we find some non-abelian first-homotopy groups to realize braiding?

Adrien Bouhon
NORDITA/Cambridge

Robert-Jan Slager
Harvard/Cambridge

Tomáš Bzdušek
Zürich

Homotopic ideas in condensed matter

- Periodic media – Bloch Hamiltonians defined on Brillouin zone:

$$H(\boldsymbol{k}) \quad \boldsymbol{k} \in T^d$$

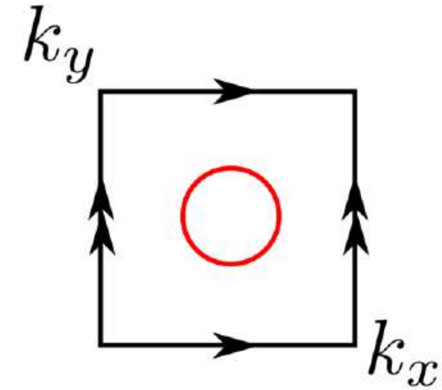
- For topology: Non-interacting, eigenstates form frame

$$|\psi_i(\boldsymbol{k})\rangle_{i \in \{1 \dots N\}} \in \frac{U(N)}{[U(1)]^N}$$

Bloch eigenstates

Ordered by energy

Homotopic ideas in condensed matter



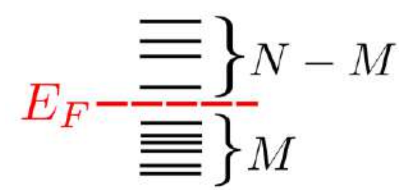
$H(\boldsymbol{k}) \quad \boldsymbol{k} \in T^d$

- Study mappings: $T^d \to U(N)/[U(1)^N]$

  - On patches in Brillouin zone: $S^{D<d} \to U(N)/[U(1)^N]$

  - Impose gap conditions (equivalence relations):

$$T^d \to \frac{U(N)}{U(N-M) \times U(M)} \simeq \mathrm{Gr}^{\mathbb{C}}_{M,N}$$



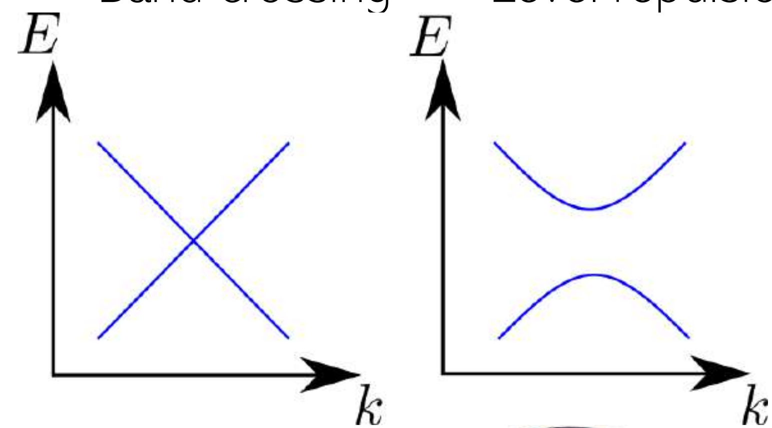
  - Impose symmetries: $U(N) \to O(N)$

Example: Weyl points

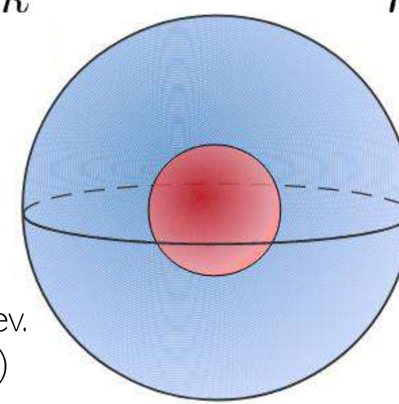
$$H(\boldsymbol{k}) \quad \boldsymbol{k} \in T^d \qquad\qquad S^{D<d} \to U(N)/[U(1)^N]$$

Specialize to two-band subspace in 3D:

$$S^2 \to \frac{U(2)}{U(1) \times U(1)}$$

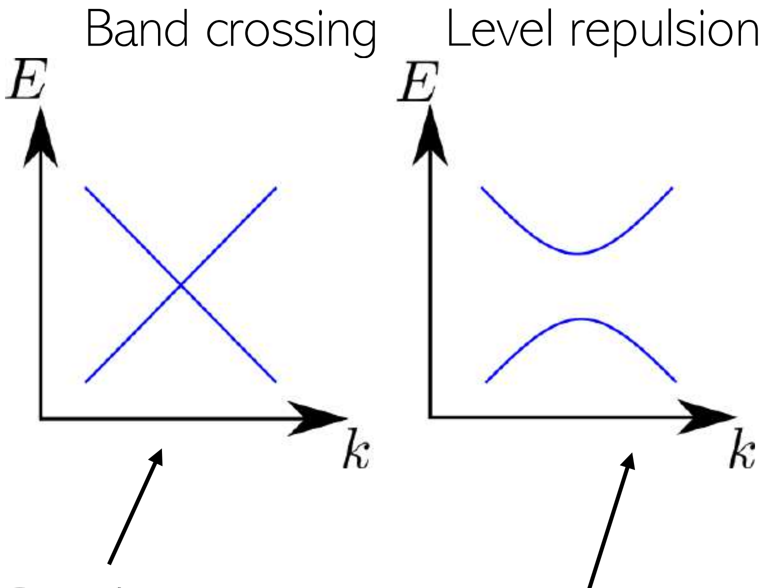


$$\pi_2 \left[\frac{U(2)}{U(1) \times U(1)} \right] = \mathbb{Z}$$



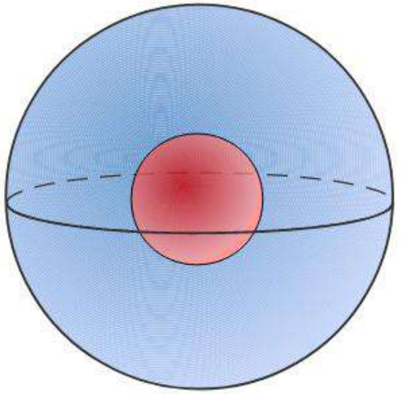
Bzdušek et al., Phys. Rev. B 96, 155105 (2017)

Example: Weyl points



$Q \neq 0$

$Q = 0$

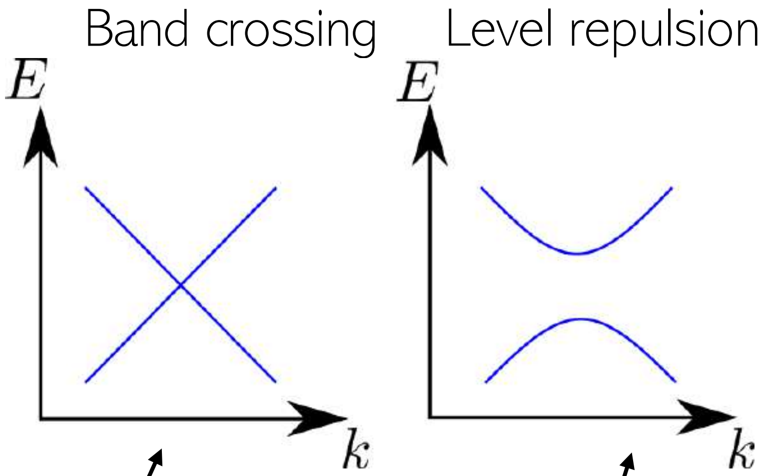


Bzdušek et al., Phys. Rev. B 96, 155105 (2017)

$$\pi_2 \left[\frac{U(2)}{U(1) \times U(1)} \right] = \mathbb{Z}$$

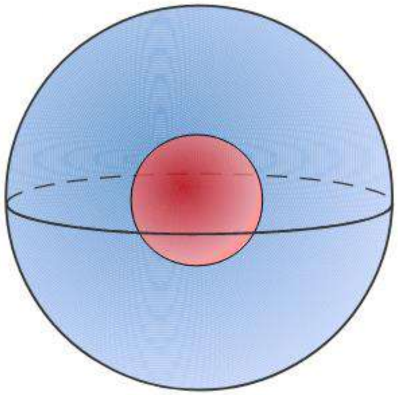
- Well defined charges
- Well-defined dispersion
- Charge conservation (Nielsen-Ninomya)

Example: Weyl points



$Q \neq 0$ $\qquad$ $Q = 0$

- Well defined charges
- Well-defined dispersion
- Charge conservation (Nielsen-Ninomya)



Bzdušek et al., Phys. Rev. B 96, 155105 (2017)

$$\pi_2 \left[\frac{U(2)}{U(1) \times U(1)} \right] = \mathbb{Z}$$

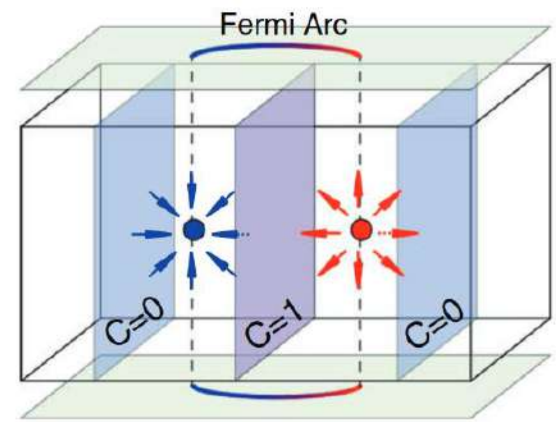
Particles in k-space!

Relationship to high-energy physics

- Various dispersions possible (not constrained by Lorentz symmetries)

- Naturally realize chiral anomaly

- More generally: Crystals have been found to host axions, higher-spin particles, etc.

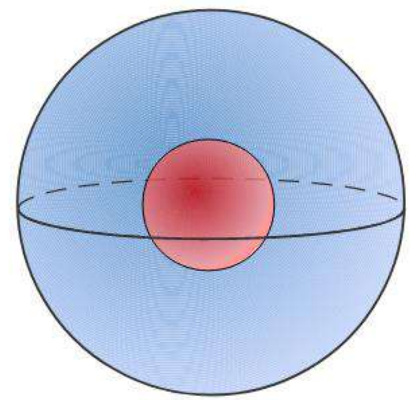


Ma et al., *Nature Communications* Volume 12, Article number: 3994 (2021)

Braiding of Weyl points?

$$\pi_1\left[\frac{U(2)}{U(1)\times U(1)}\right]=\mathbb{0}$$

No non-trivial braiding



Bzdušek et al., Phys. Rev. B 96, 155105 (2017)

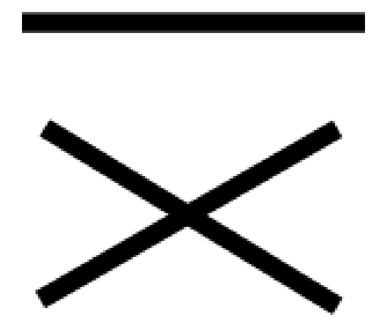
$$\pi_1\left[\frac{\mathrm{SO}(3)}{S[\mathrm{O}(2)\times \mathrm{O}(1)]}\right]=\mathbb{Z}_2$$

Quaternion group – Non-abelian!

$$\pi_1\left[\frac{\mathrm{SO}(3)}{S[\mathrm{O}(1)\times \mathrm{O}(1)\times \mathrm{O}(1)]}\right]=\mathbb{Q}$$

Multi-gap topology

$$\pi_1\left[\frac{\mathrm{SO}(3)}{S[\mathrm{O}(2)\times\mathrm{O}(1)]}\right]=\mathbb{Z}_2$$



2+1 bands, symmetry making eigenstates real

$$\pi_1\left[\frac{\mathrm{SO}(3)}{S[\mathrm{O}(1)\times\mathrm{O}(1)\times\mathrm{O}(1)]}\right]=\mathbb{Q}$$

1+1+1 bands (multi-gap), symmetry making eigenstates real

Reality condition

$$\pi_1\left[\frac{\mathrm{SO}(3)}{S[\mathrm{O}(1)\times\mathrm{O}(1)\times\mathrm{O}(1)]}\right]=\mathbb{Q}$$

1+1+1 bands (multi-gap), symmetry making eigenstates real

$$C_2: \quad H(\boldsymbol{k}) = U_{C_2} H(C_2\boldsymbol{k}) U_{C_2}^\dagger$$

$$\mathcal{I}: \quad H(\boldsymbol{k}) = U_{\mathcal{I}} H(-\boldsymbol{k}) U_{\mathcal{I}}^\dagger$$

$$\mathcal{T}: \quad H(\boldsymbol{k}) = U_{\mathcal{T}} H(-\boldsymbol{k})^* U_{\mathcal{T}}^\dagger$$

Spin even/odd

$$[C_2\mathcal{T}]^2 = +1 \qquad [\mathcal{I}\mathcal{T}]^2 = \pm 1$$

Reality condition

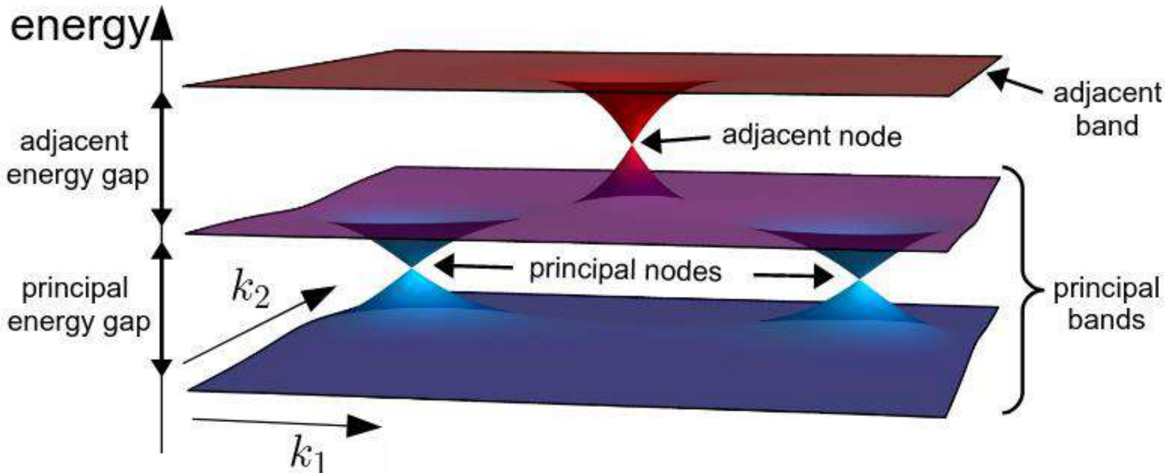
$$\pi_1\left[\frac{\mathrm{SO}(3)}{S[\mathrm{O}(1)\times\mathrm{O}(1)\times\mathrm{O}(1)]}\right]=\mathbb{Q}$$

1+1+1 bands (multi-gap), symmetry making eigenstates real

Even spin and $\mathcal{I}\mathcal{T} \longrightarrow H(\boldsymbol{k})$ real everywhere

Any spin and $C_2\mathcal{T} \longrightarrow H(\boldsymbol{k})$ real in plane

Braiding Weyl points

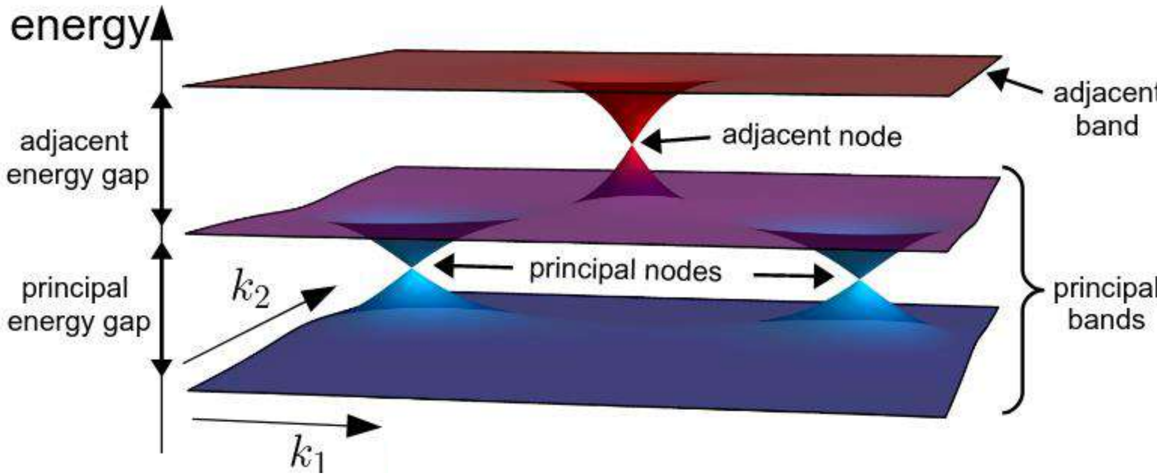


Bouhon et al. *Nature Physics* volume 16, pages 1137–1143 (2020)

Multi-gap states in $C_2\mathcal{T}$ –invariant plane in k-space

Characterized by Quaternion group!

Quaternion group



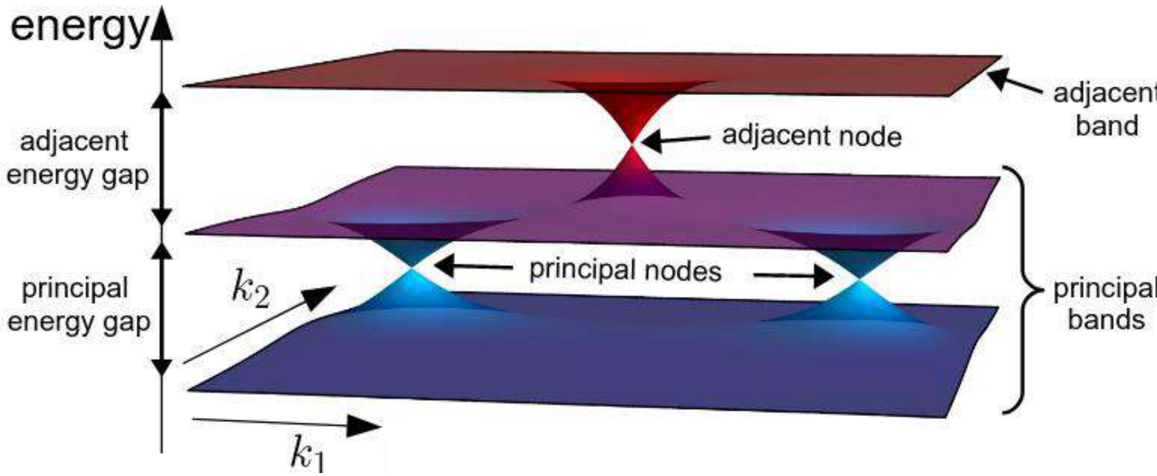
Bouhon et al. *Nature Physics* volume 16, pages 1137–1143 (2020)

Physically:
- i: Node in first gap
- j: Node in both gaps
- k: Node in second gap
- -1: Double node

Braiding between nodes in different gaps!

	1	i	j	k
1	1	i	j	k
i	i	−1	k	−j
j	j	−k	−1	i
k	k	j	−i	−1

Quaternion group



Bouhon et al. *Nature Physics* volume 16, pages 1137–1143 (2020)

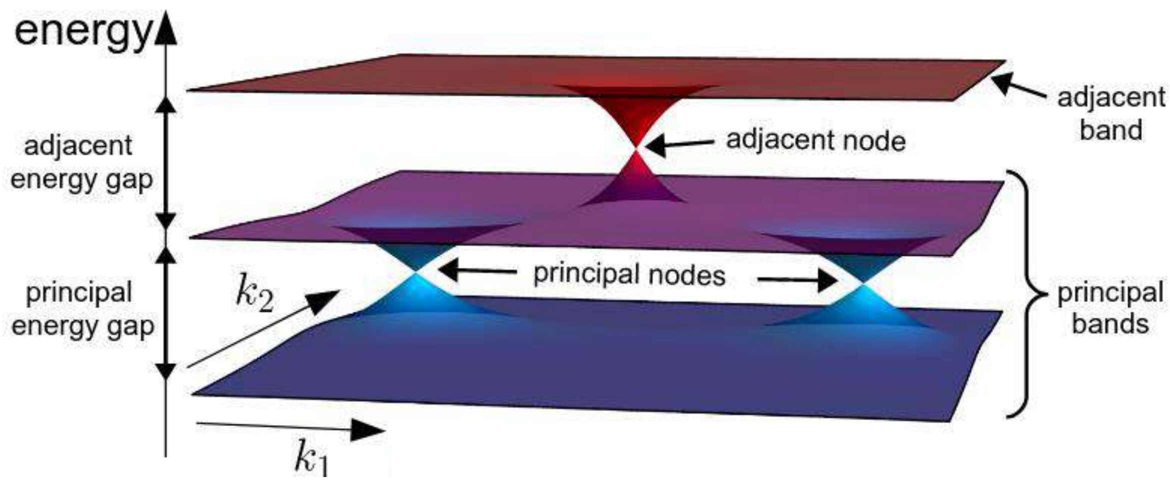
$$\mathbb{Q} = \{\pm 1, \pm i, \pm j, \pm k\}$$

$$ij = k \neq ji = -k$$

Non-abelian braiding!

	1	**i**	**j**	**k**
1	1	i	j	k
i	i	−1	k	−j
j	j	−k	−1	i
k	k	j	−i	−1

Braiding Weyl points



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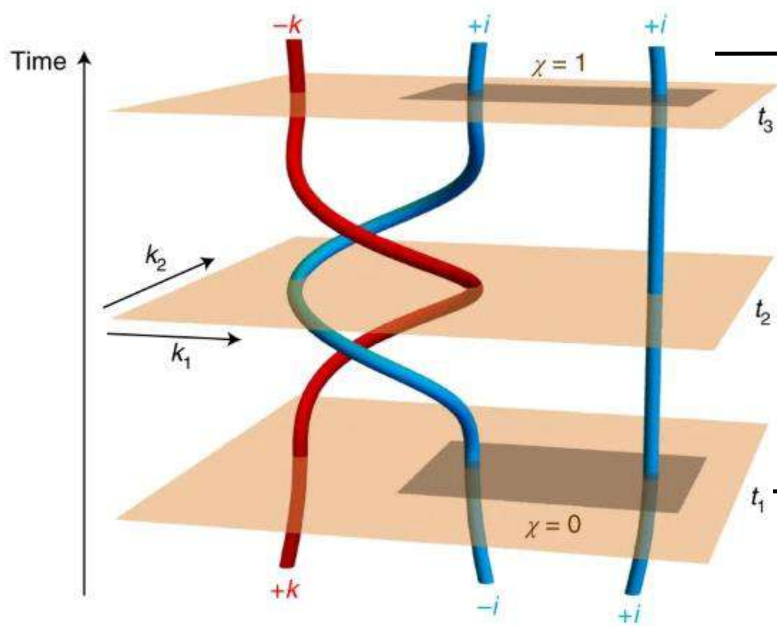
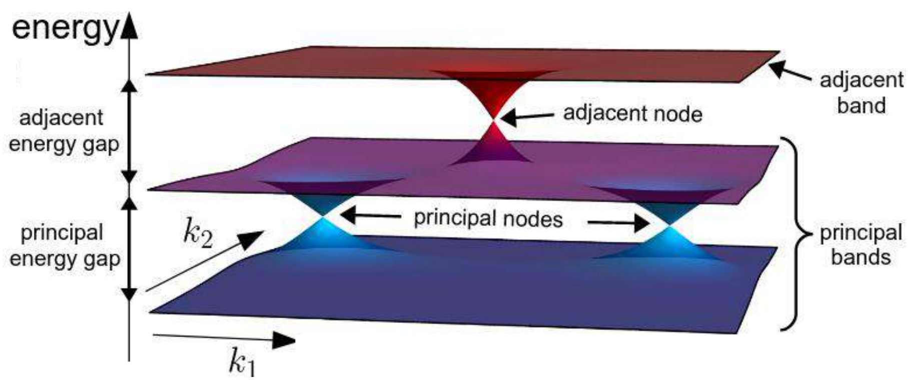
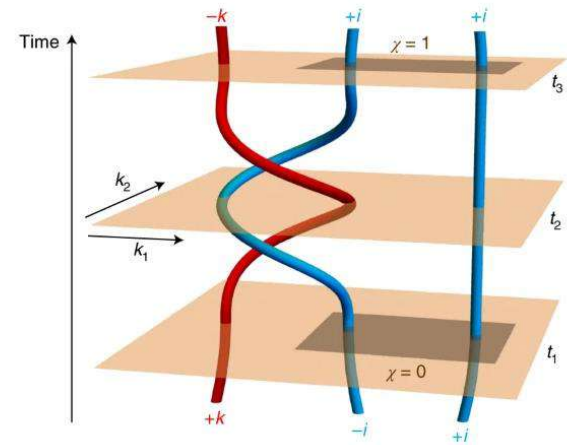


Weyl points cannot annihilate

Weyl points can annihilate

Braiding Weyl points





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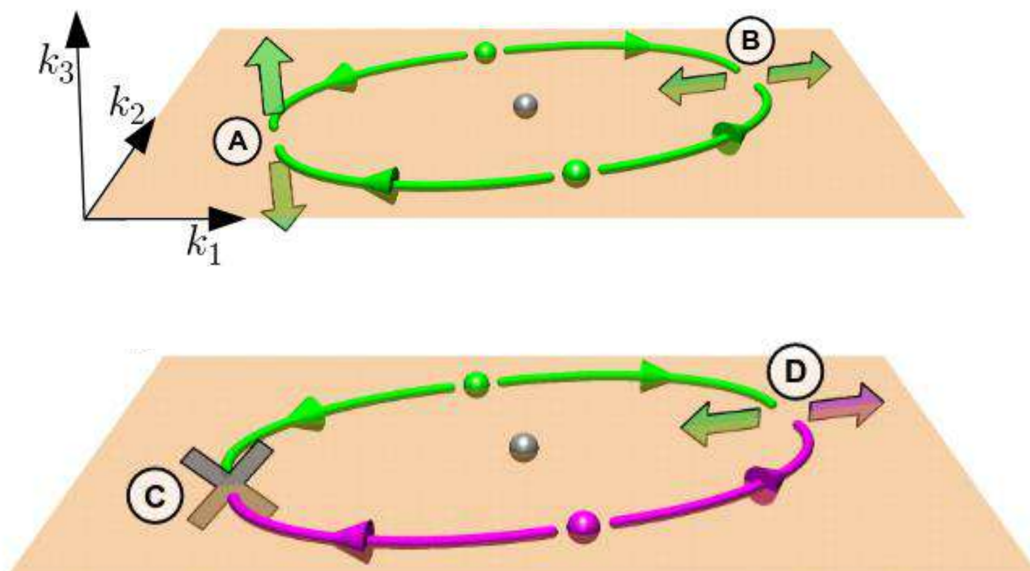
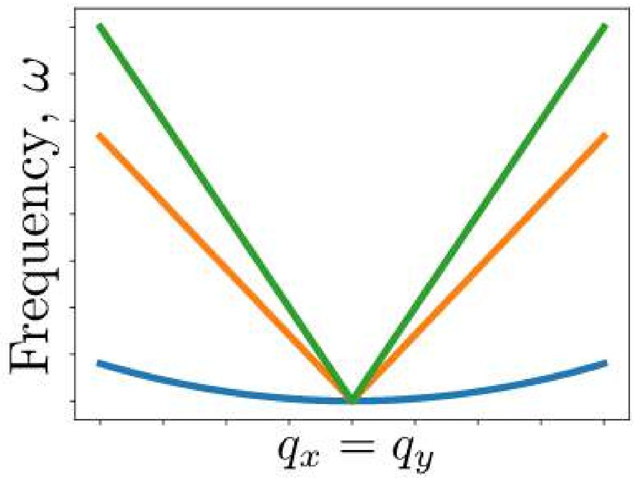


Application: Acoustic phonons in 2D

Vibrations of atoms (phonons): $D(\boldsymbol{q})v(\boldsymbol{q}) = \omega^2(\boldsymbol{q})v(\boldsymbol{q})$

Dynamical matrix
- Positive semi-definite
  - Local inversion symmetry

Phonon eigenstates
- Spin-0
- Automatically time-reversal invariant

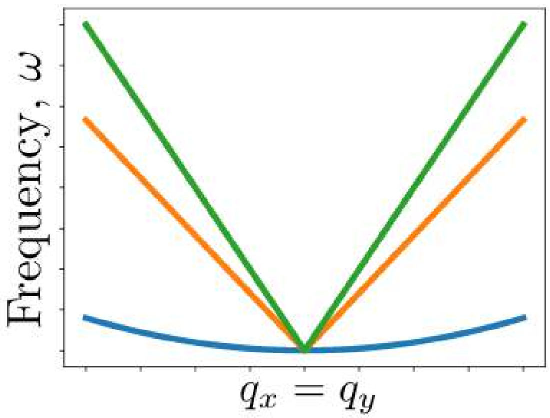


Lange et al., Phys. Rev. B **105**, 064301 (2022)

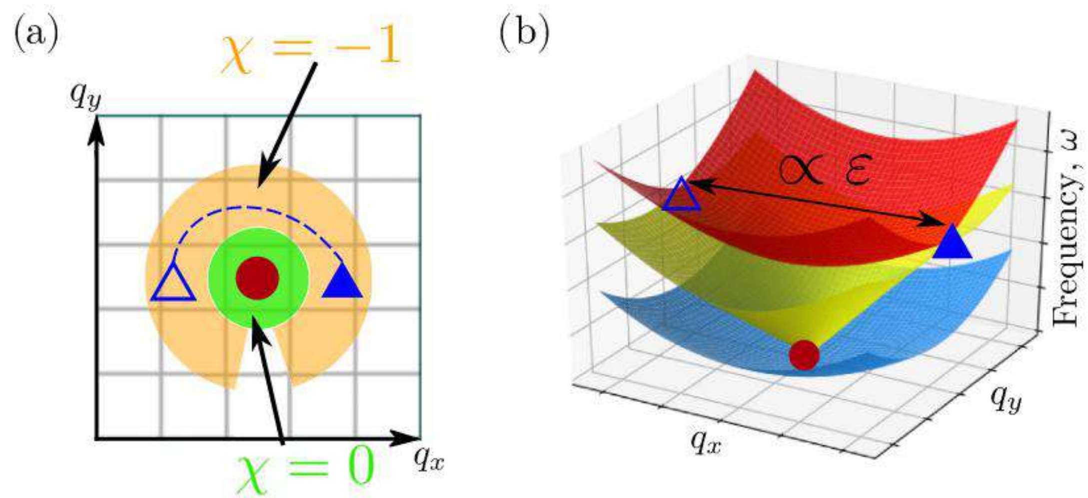
Low-q dispersion in 2D
- Acoustic phonons (Goldstone bosons)
- 2 linear modes & 1 quadratic mode (flexural)

Charge?

Application: Acoustic phonons in 2D



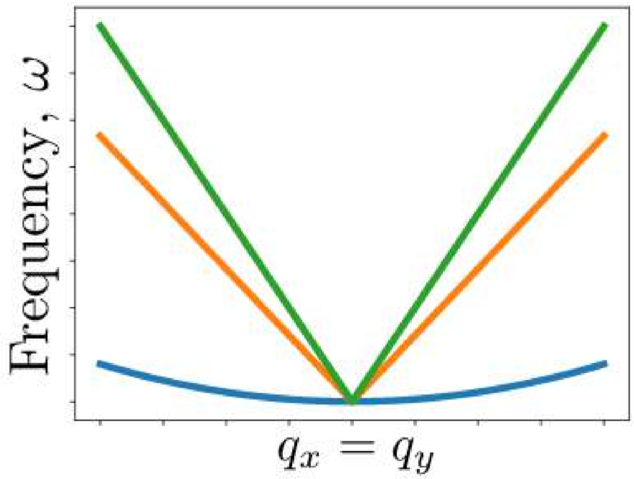
Artificially split degeneracies



Lange et al., Phys. Rev. B **105**, 064301 (2022)

Nodes characterized by Quaternions

Application: Acoustic phonons in 2D

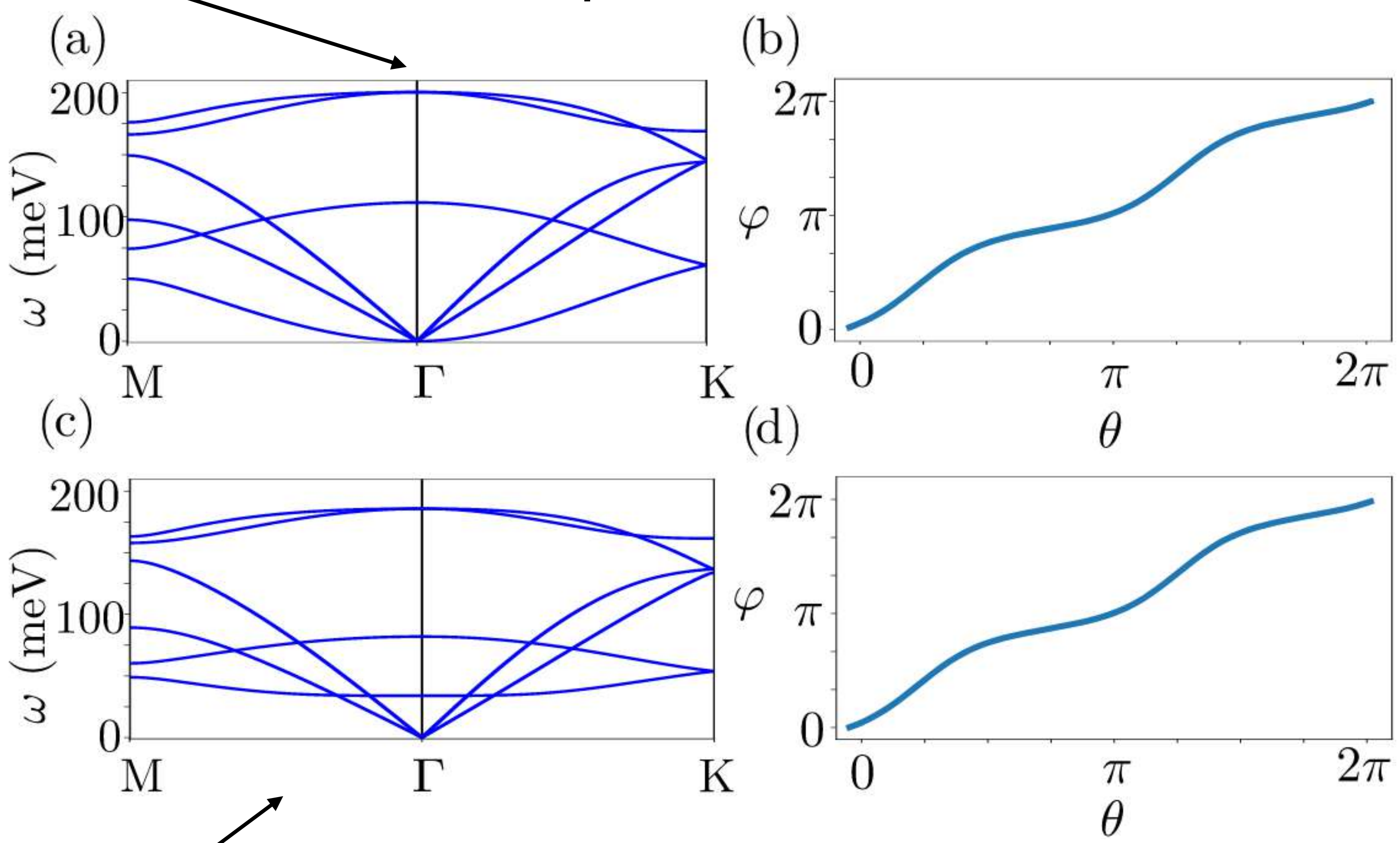


Lange et al., Phys. Rev. B **105**, 064301 (2022)

Caveat: If system has $\mathcal{I}$ and $\mathcal{T}$ separately, possible charges at triple-point are ± 1

Application: Acoustic phonons in Graphene

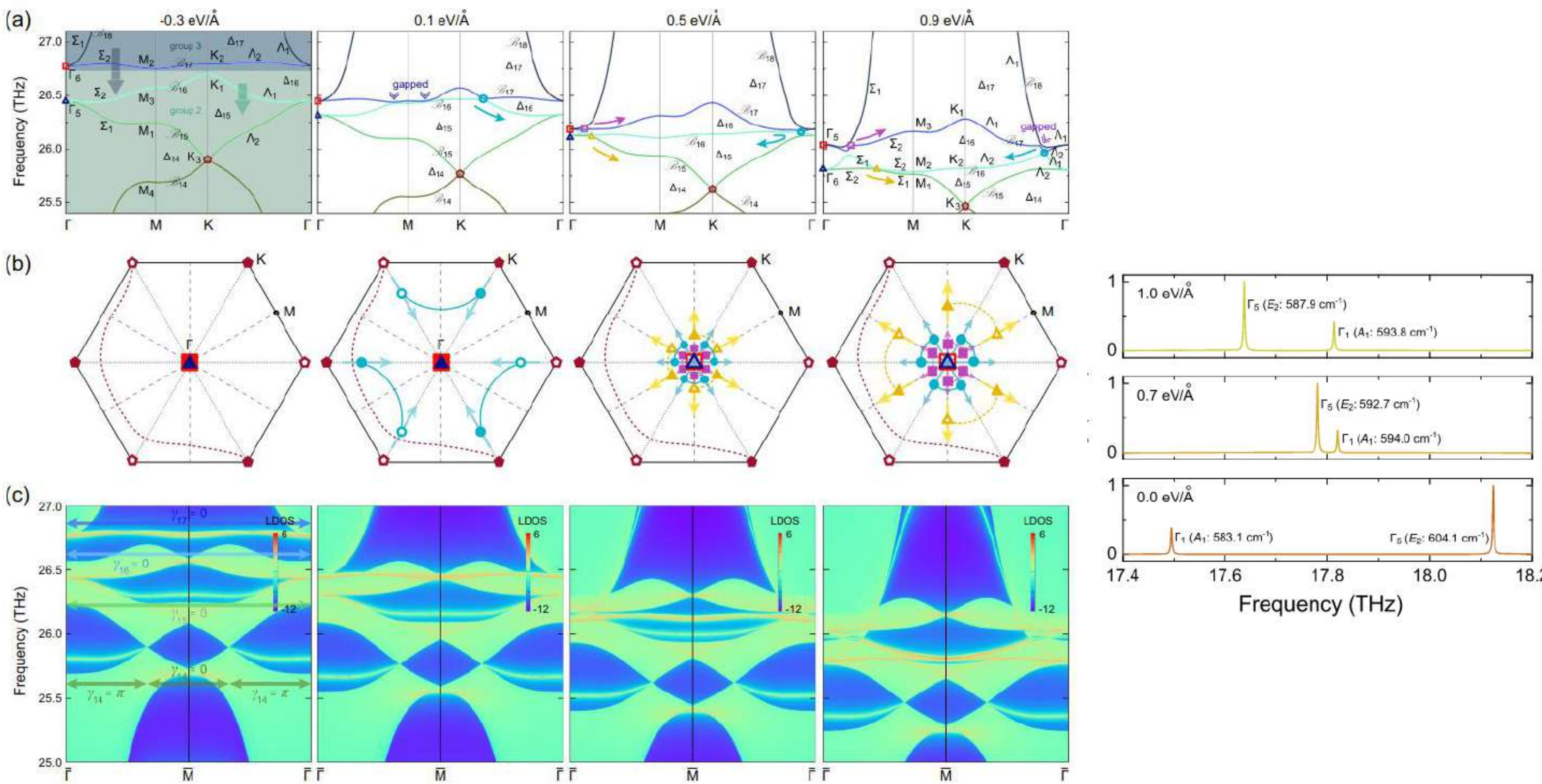
Free standing



On substrate

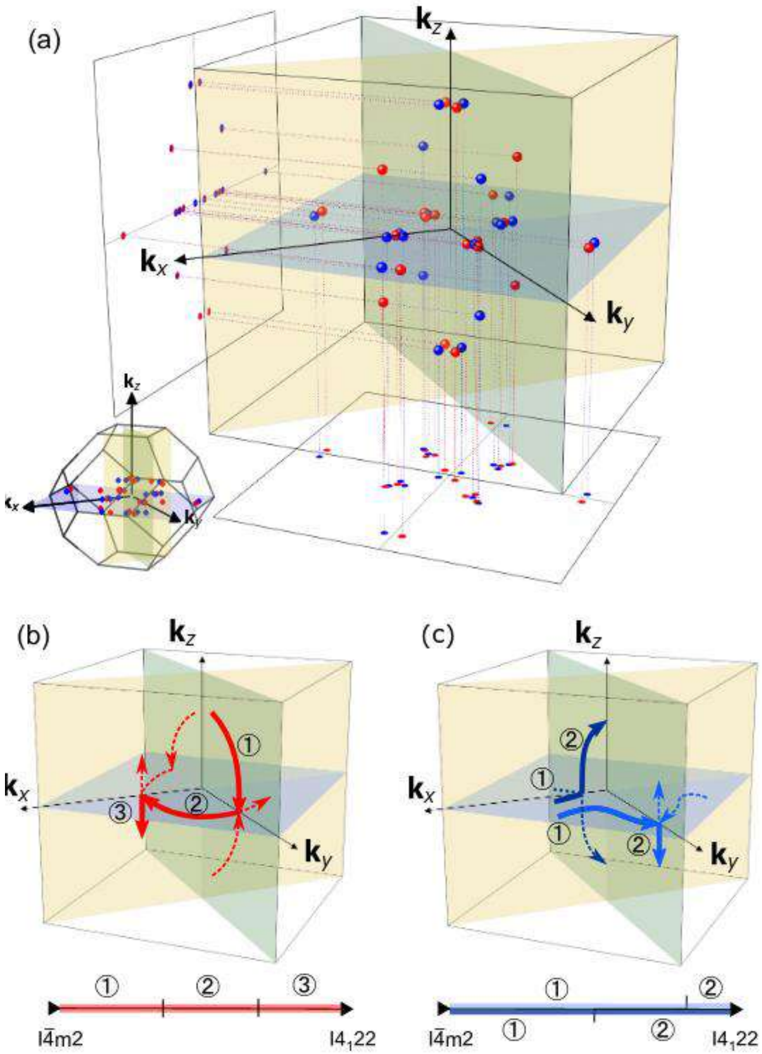
Lange et al., Phys. Rev. B **105**, 064301 (2022)

Application: Phonons manipulated by electric field in silicates



Peng et al., Nature Communications volume 13, Article number: 423 (2022)

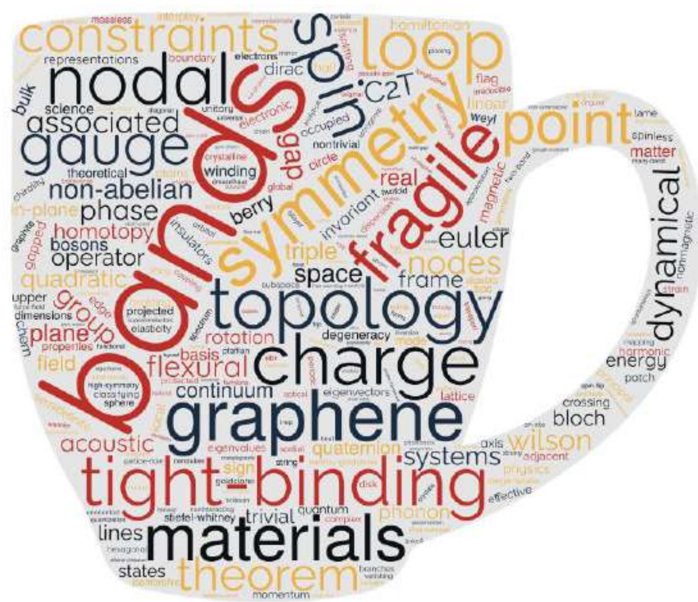
Application: Electron phase transitions manipulated by temperature in $Cd_2Re_2O_7$



Chen et al., Phys. Rev. B **105**, L081117 (2022)

Conclusion/Outlook

- Many topological phases in band structures
- Weyl points feature interesting physics
- Multi-gap topology can interact with Weyl points
- Exists in phonons and electrons
- Lots of exciting things to come!



TCM

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Cambridge

Siyu Chen
Cambridge

Dominik Hamara
Cambridge

Chiara Ciccarelli
Cambridge

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GFL25@CAM.AC.UK