Localization and interactions in topological bands

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Talk at the Nordita Conference on
Quantum Engineering of States *and Devices*,
August 20, 2014

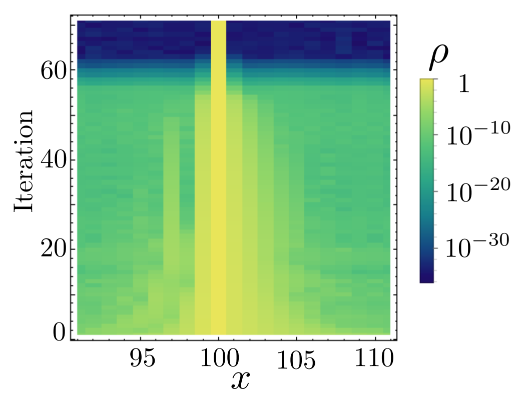
This talk

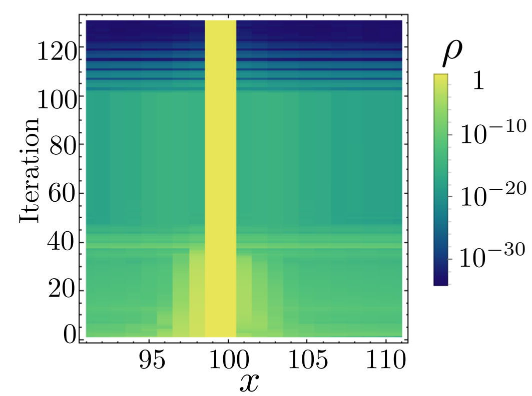
- Impact of topology on localization

  - Fundamental restrictions on Wannier functions

  - Compressed sensing approach to finding most localized representative of a topological phase

J.C. Budich, J. Eisert, E.J. Bergholtz, S. Diehl, and P. Zoller arXiv:1405.6641





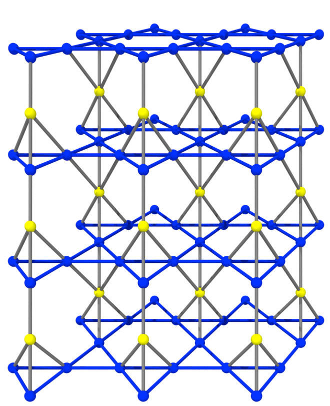
- Impact of localization on topology!

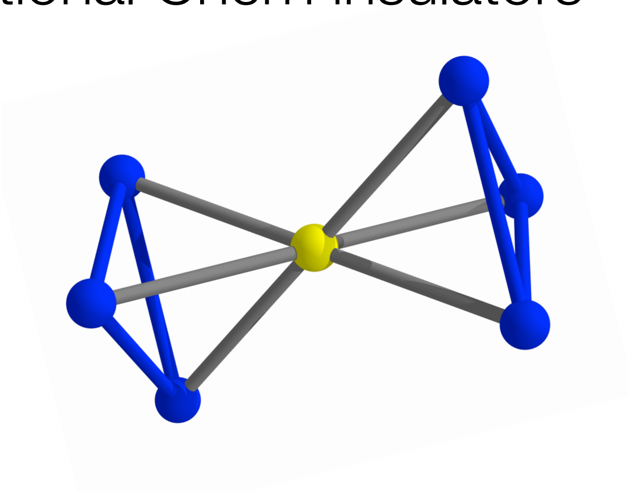
  - From Weyl semi-metals and Fermi arcs to fractional Chern insulators

E.J. Bergholtz, Z. Liu, M. Trescher, R. Moessner, and M. Udagawa arXiv:1408.3669

M. Trescher and E.J. Bergholtz Phys. Rev. B 86, 241111(R) (2012)

Z. Liu, E.J. Bergholtz, H. Fan, A. M. Läuchli Phys. Rev. Lett. 109, 186805 (2012)





Key ingredients:

spin-orbit coupling,
geometrical frustration,
interactions

Impact of topology on localization:

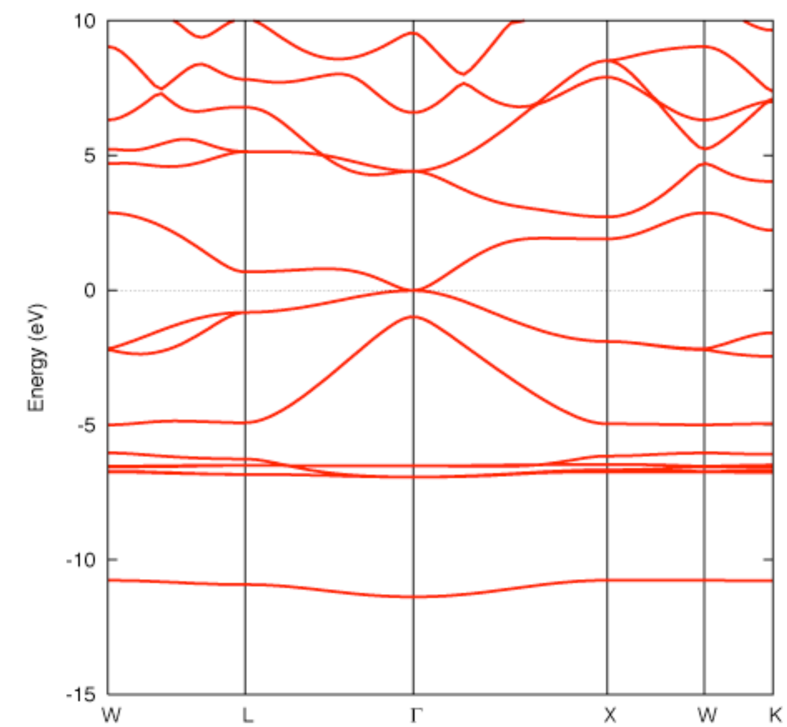
Wannier functions

Bloch states and Wannier functions

- How do we suitably represent the single particle states in a solid efficiently?

  - Depends on what we want to investigate.

  Two natural choices:



(Band structure of HgTe)

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

- Eigenstates with energy $E_{\mathbf{k}}$
- Delocalized (in real-space)

Wannier functions $$w_{\mathbf{R}}^{\alpha}(\mathbf{r}) = \sum_{\mathbf{k}} e^{-i\mathbf{k}\cdot\mathbf{R}} \psi_{\mathbf{k}}^{\alpha}(\mathbf{r})$$

- Not eigenstates (except for flat bands), but span the same space as the Bloch states
- Local in real-space...
- But not uniquely defined!

$$\psi_{\mathbf{k}}^{\alpha}(\mathbf{r}) \to \sum_{\beta=1}^{N_{\text{bands}}} U_{\alpha\beta}(\mathbf{k}) \psi_{\mathbf{k}}^{\beta}(\mathbf{r})$$

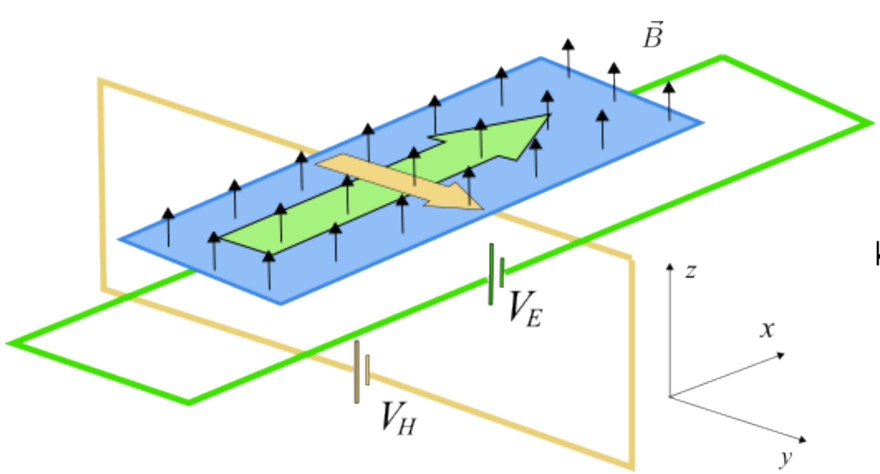
Smooth unitary transf,

How localized *can* the Wannier functions possibly be?

- Kohn (1959): In one dimension, exponentially localized Wannier functions always exist
  - Decay lengths depend details
- Thouless (1984): In Landau levels, the Wannier functions cannot decay quicker than $\sim r^{-2}$

  (Asymmetric choices possible, e.g., $\sim e^{ikx} e^{-(y-k)^2/2}$)

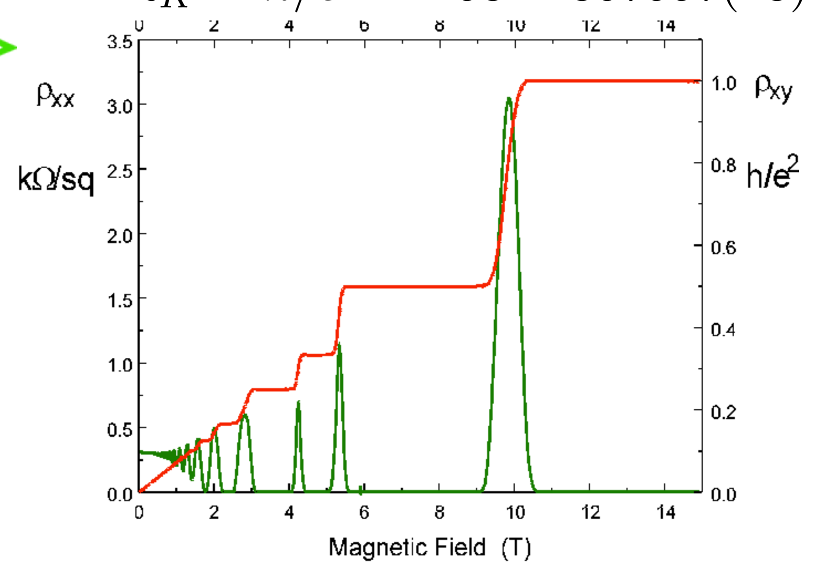
Quick recap: Landau levels

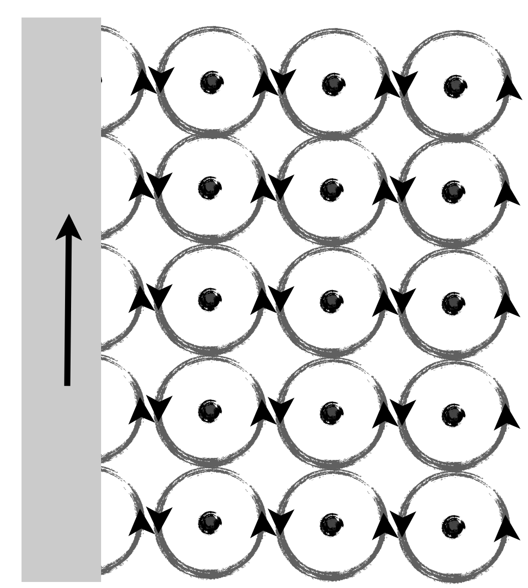


(von Klitzling et al '80)

Quantization, IQHE:

$R_K = h/e^2 = 25812.807557(18)\Omega$





Chern number

(Thouless et al '82)

How localized *can* the Wannier functions possibly be?

- General statement: exponentially localized Wannier functions if and only if the (total) Chern number vanish.

  - Non-zero Chern number as an obstruction for a smooth global gauge.

  See e.g., Brouder et. al. Phys. Rev. Lett. 98, 046402 (2007)

  - Quantum spin Hall (QSH) insulators have exponential Wannier functions, even in the limit of two time-reversed Chern insulators!

- How about strictly localized (compact) Wannier functions?

  - Not covered by the above considerations.

  - If existing, they directly provide local dispersionless “sweet spot” models.

$$H = -\sum_{i,\alpha} w^{\dagger}_{i,\alpha} w_{i,\alpha}$$

Example: Kitaev chain $$w_j = (c_j + c_j^{\dagger} - c_{j+1} + c_{j+1}^{\dagger})$$

How to actually find “maximally” localized Wannier functions?

- Standard approach: (initial guess +) gradient search

N. Marzari, D. Vanderbilt, Phys. Rev. B 56, 12847 (1997)

  - Very successful
  - Heavily used in first principles applications

- Ozolins et al., (2013): Use compressed sensing!

Ozolins et al., PNAS 110, 18368 (2013)

  - Novel approach using ideas of contemporary mathematics and image processing
  - Iteratively minimize on a finite lattice $\mathcal{E}(\psi) + \frac{1}{\xi}\|\psi\|_\rho$

Energy (expectation value)

real number, decides relative priorities

l_1-norm, favors localized states

- We generalized the algorithm as to preserve symmetries, e.g., time-reversal, charge conjugation etc.

J.C. Budich, J. Eisert, E.J. Bergholtz, S. Diehl, and P. Zoller arXiv:1405.6641

  - Crucial for any application to topological states!
  - Gives a search algorithm for “sweet spots” as $\xi \to 0$

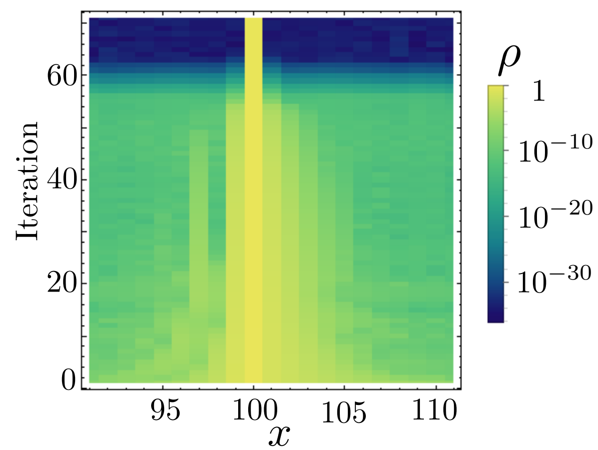
- We also achieve a significant speedup of the significant algorithm

Performance: examples and a conjecture

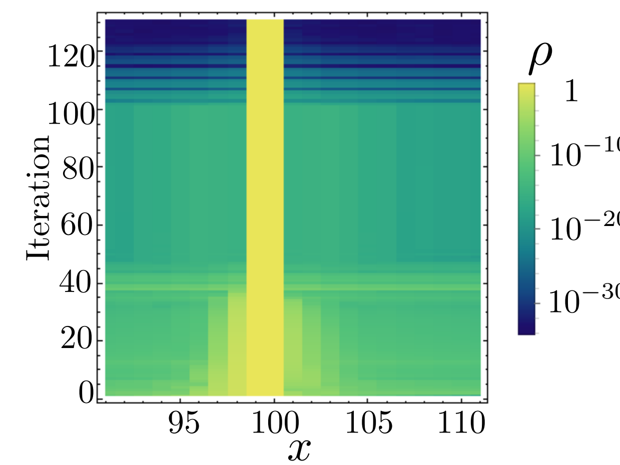
- We start with a random representatives of various topological classes and let $\xi \to 0$

- 1D superconductors

  - "Trivial" case: converge quickly to Wannier functions localized on a single site



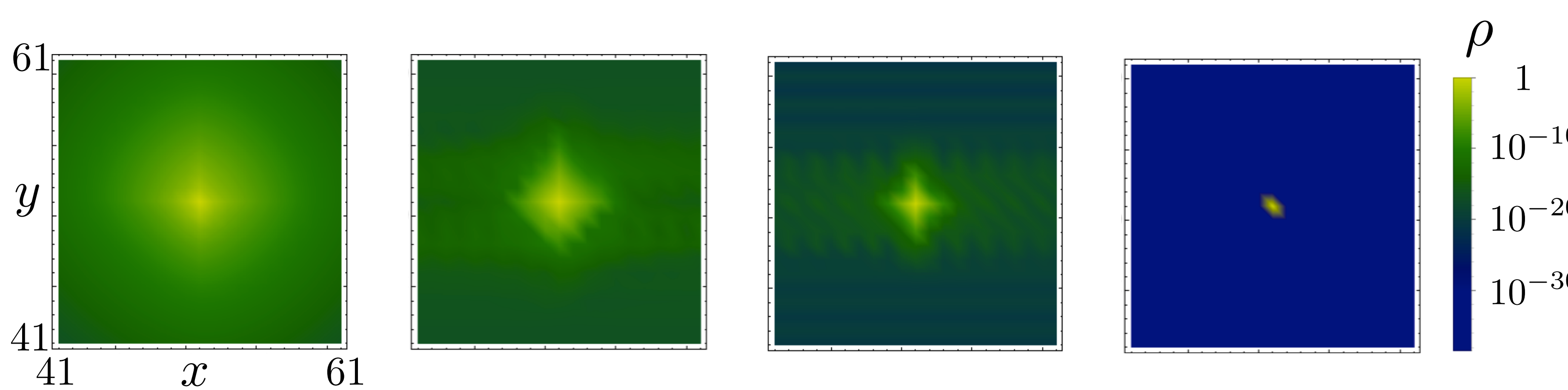
  - Topological case: converge to the known Kitaev case!



- 2D topologically trivial states

  - Works extremely well

  - Here, a 101x101 lattice and 727 iterations, can be easily done on a laptop



- But: for the QSH the algorithm does not converge -- any truncation breaks the symmetries at the "same order".

  - <u>Conjecture</u>: no "sweet spot" exists for the quantum spin Hall effect

Impact of localization on topology:

From *Weyl semi-metals* and *Fermi arcs* to *fractional Chern insulators*

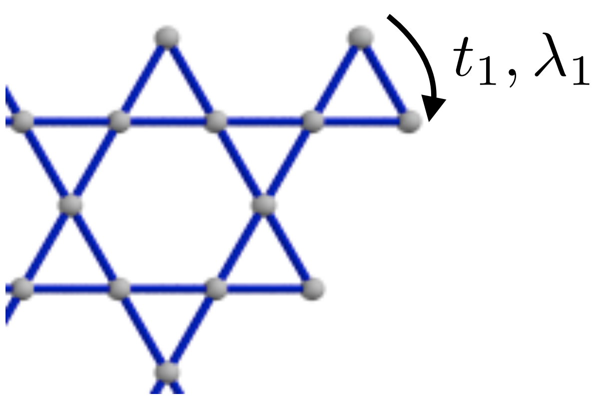
Topological Flat Band Models and Fractional Chern Insulators

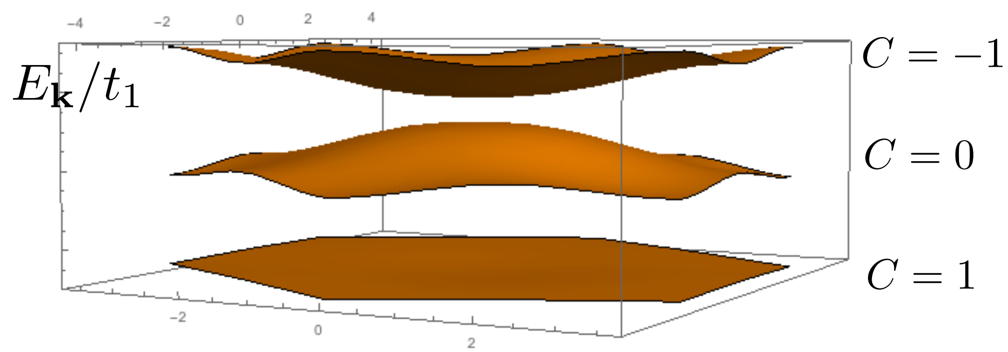
- Important insight:

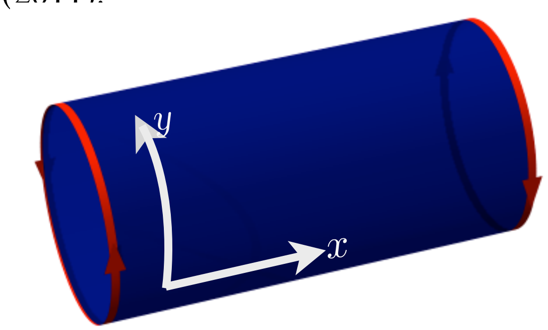
  - Lattice analogues of Landau levels, flat topological Chern bands, can form in e.g, spin-orbit coupled systems in presence of ferromagnetism.

Complex history, recently turned into mainstream since

E. Tang, J.-W. Mei, and X.-G. Wen, Phys. Rev. Lett. **106**, 236802 (2011).
K. Sun, Z. Gu, H. Katsura, and S. Das Sarma, Phys. Rev. Lett. **106**, 236803 (2011).
T. Neupert, L. Santos, C. Chamon, and C. Mudry, Phys. Rev. Lett. **106**, 236804 (2011).







- Topologically protected gapless chiral edge states

- Interaction scale set by lattice spacing $\Rightarrow \Delta E \sim 500K$!?

- Zero external magnetic field!

- Theory: interactions lead to “fractional Chern insulators” (FCIs)

  - Qualitatively new challenges and possibilities arise due to the interplay between (band) topology, interactions and the lattice.

Review: **Topological Flat Band Models and Fractional Chern Insulators**
E.J. Bergholtz and Z. Liu, *Int. J. Mod. Phys. B 27, 1330017 (2013).*

Something qualitatively new: Flat C>1 bands

M. Trescher and E.J. Bergholtz,
Phys. Rev. B 86, 241111(R) (2012)

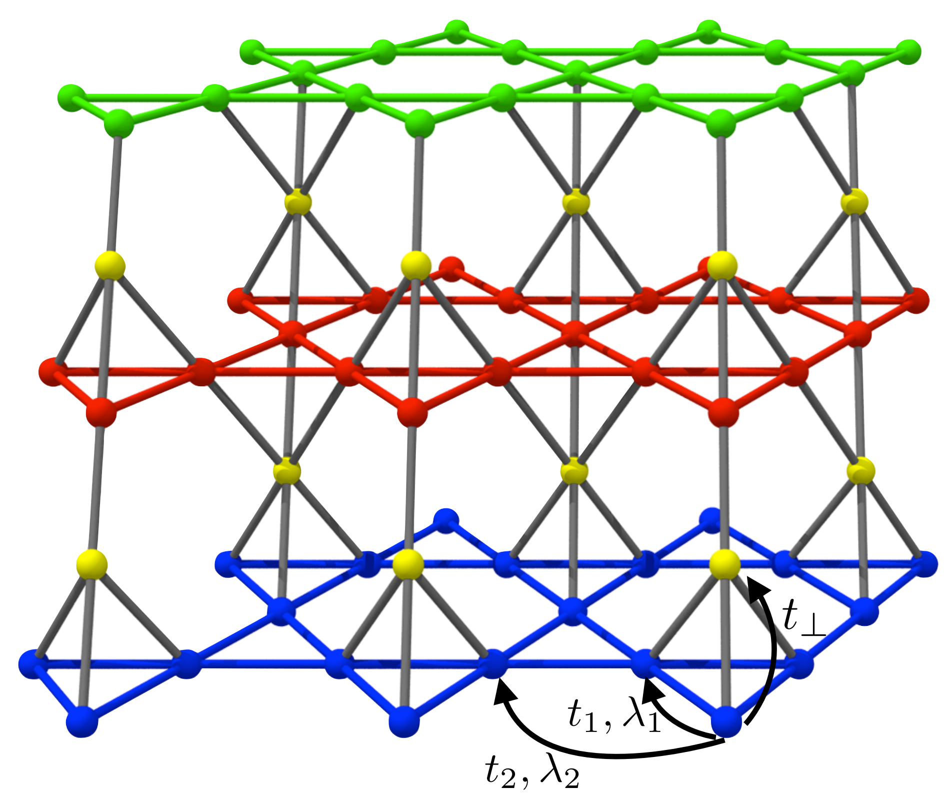
- We ask: Is it possible to make N C=1 bands hybridize so that one band absorbs all the topology (C=N) while the others become trivial (C=0)?

$$1 + 1 \rightarrow 2 + 0?$$

- Our answer: yes, using
  - Multilayer systems
  - Geometrical frustration

- We implement our idea on pyrochlore slabs inspired by pyrochlore based spin-orbit coupled materials, e.g. iridates.

$$H = \sum_{i,j,\sigma} t_{ij} c^\dagger_{i\sigma} c_{j\sigma} + i \sum_{i,j,\alpha,\beta} \lambda_{ij} (\mathbf{E}_{ij} \times \mathbf{R}_{ij}) \cdot \boldsymbol{\sigma}_{\alpha\beta} c^\dagger_{i\alpha} c_{j\beta}$$

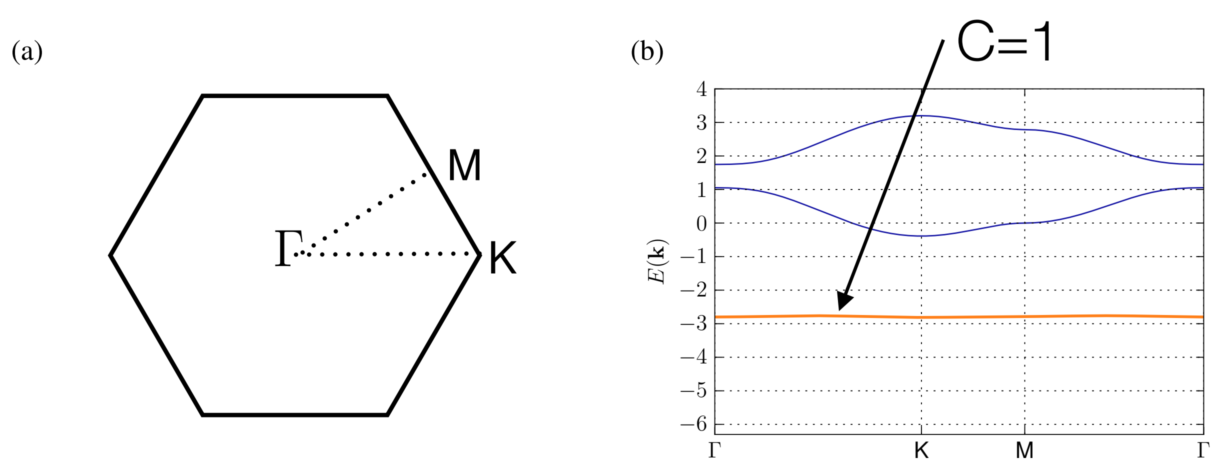


- Note: no interlayer tunneling give N degenerate C=1 bands -- this is *not* what we look for.

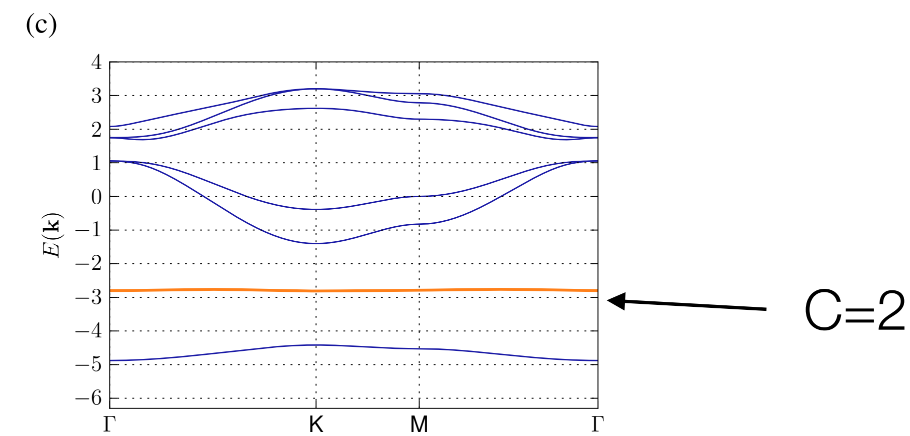
Results: 2d bulk dispersion

M. Trescher and E.J. Bergholtz,
Phys. Rev. B 86, 241111(R) (2012)

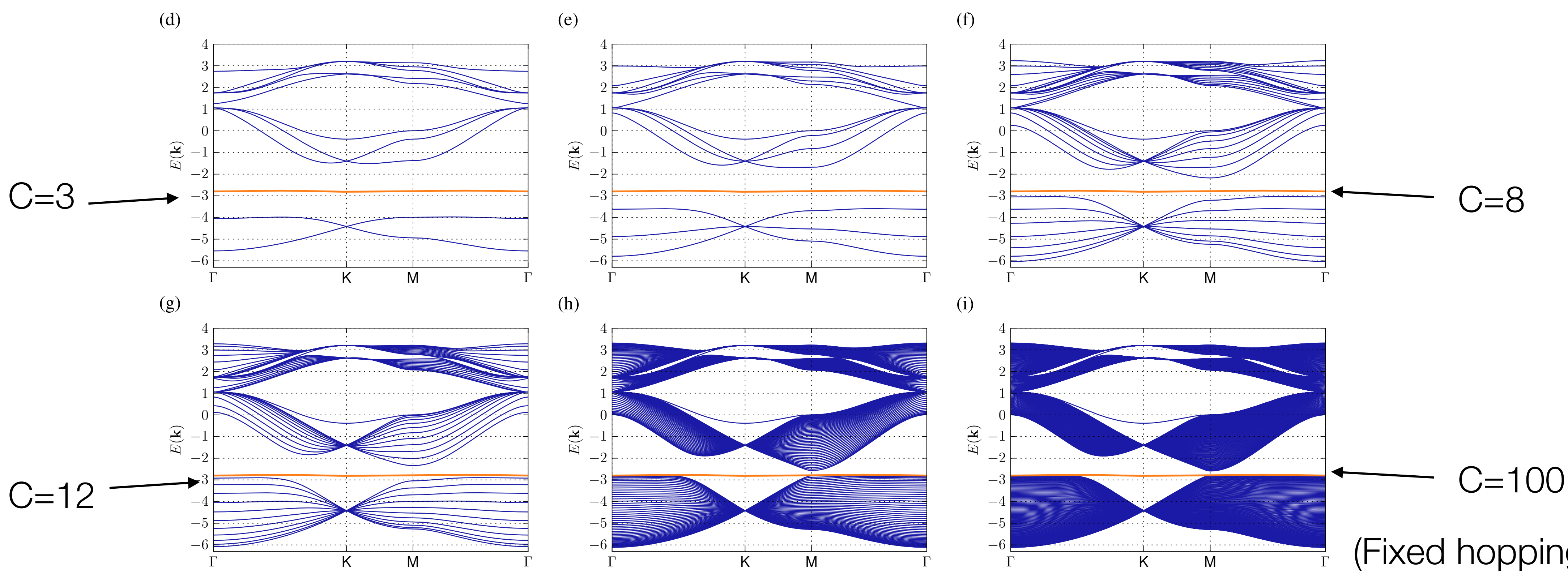
- Dispersion for one layer



- Dispersion with two layers



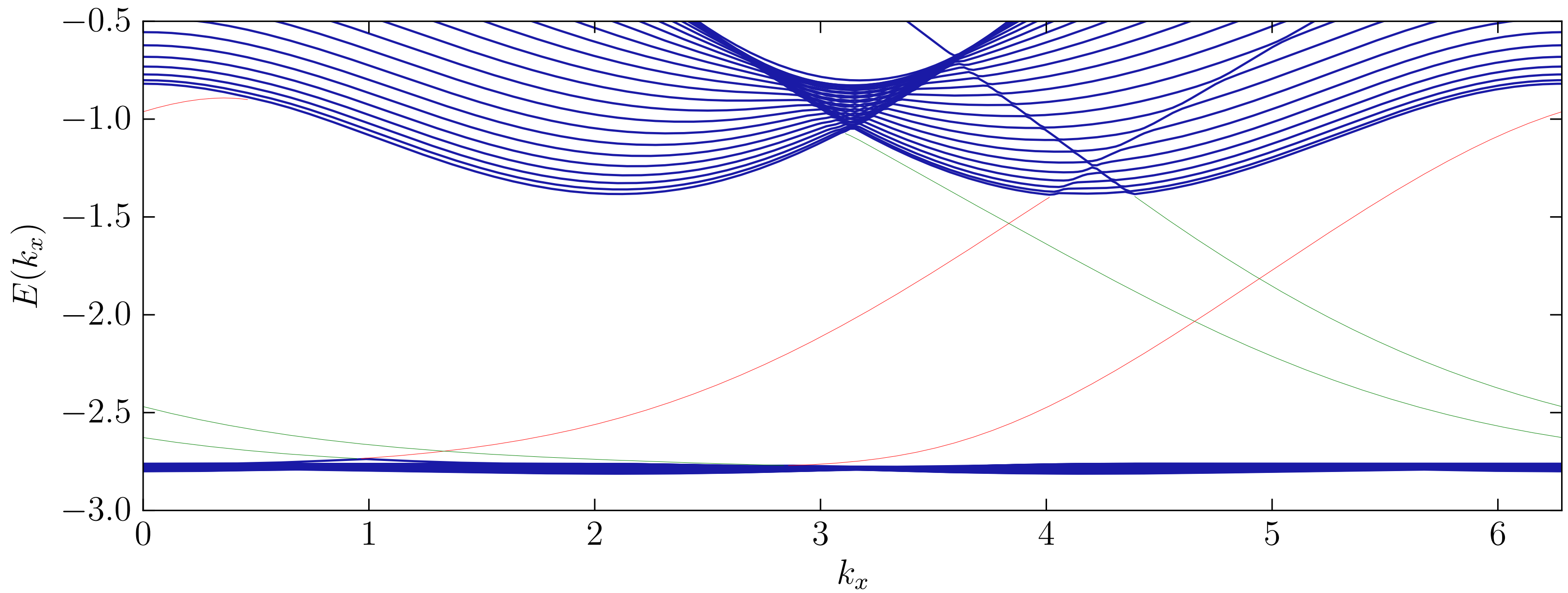
- For N kagome layers we find a flat band with C=N!

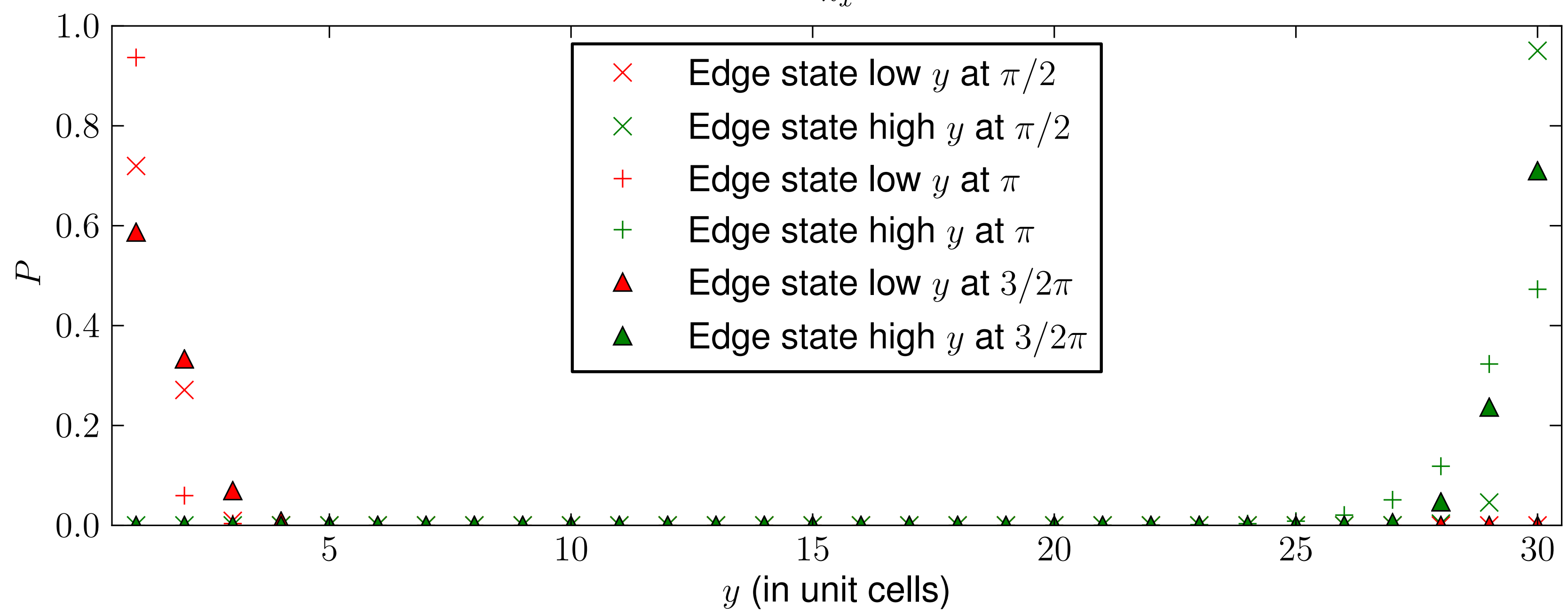


(Fixed hopping parameters here, just changing N)

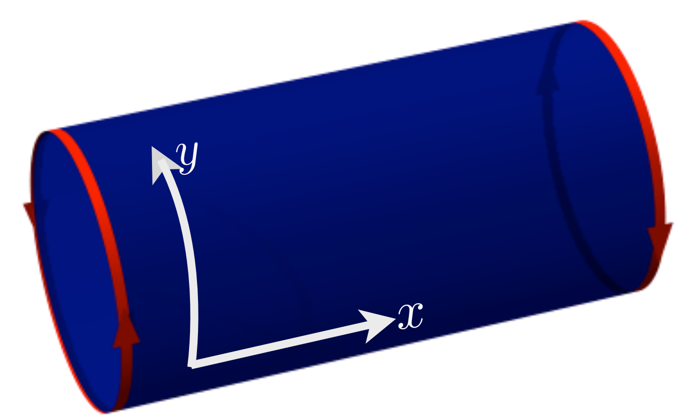
1d edge states: revealed in cylinder geometry

- Example: the C=2 band has 2 gapless chiral edge states at each end





(Microscopically different edges to avoid deceiving degeneracies)

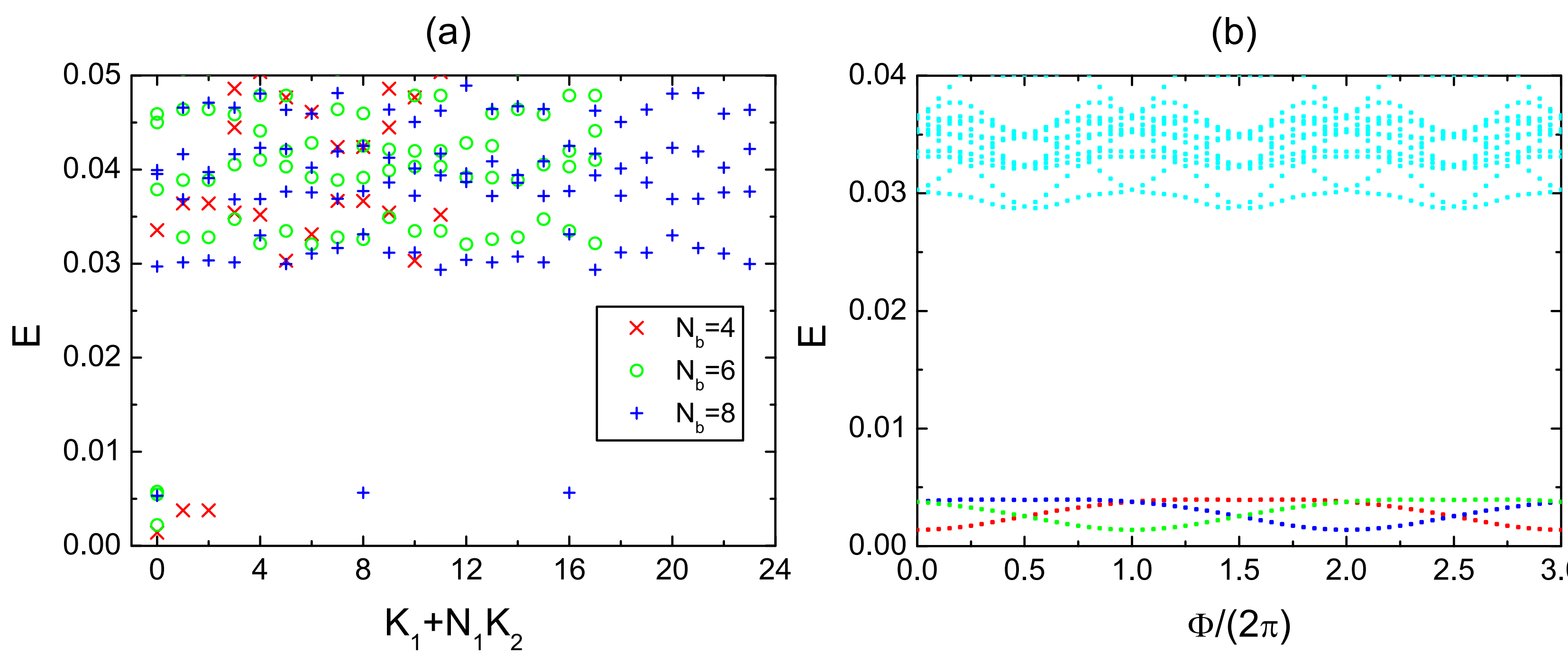


Can qualitatively new FCI phases form within C>1 bands?

Z. Liu, E.J. Bergholtz, H. Fan, A. M. Läuchli
Phys. Rev. Lett. 109, 186805 (2012)

- Yes, we find convincing evidence for a series of bosonic FCI states at $\nu_b = 1/(C+1)$

$C = 2, \nu_b = 1/3:$



- Fermionic states at $\nu_f = 1/(2C+1)$ (likely absent at higher filling fractions!)

- Strong evidence also for C>1 generalizations of non-Abelian FQH states found in this model!

E.J. Bergholtz, Z. Liu, M. Trescher, R. Moessner, and M. Udagawa, arXiv:1408.3669

A. Sterdyniak, C. Repellin, B.A. Bernevig, and N. Regnault, Phys. Rev. B 87, 205137 (2013)

- Different from standard multi-layer systems...

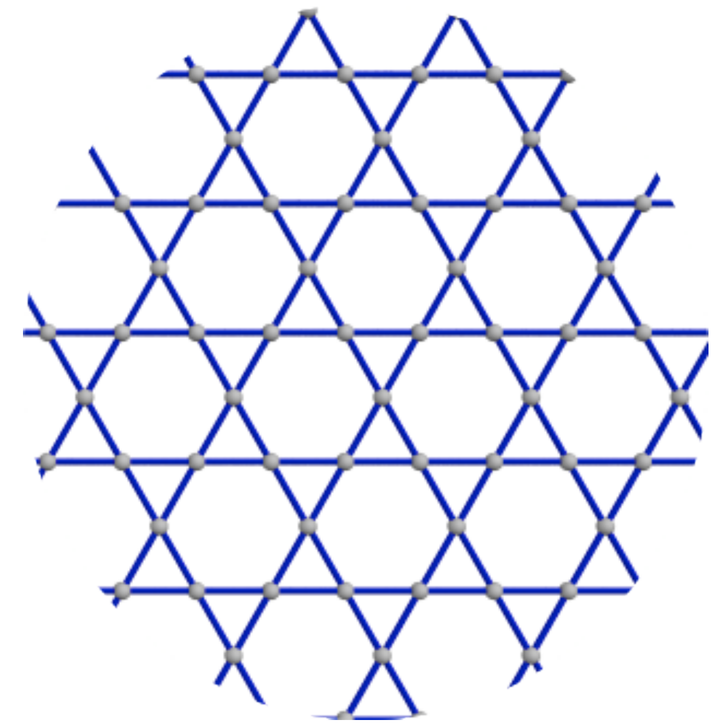
Can we analytically understand the C=N states?

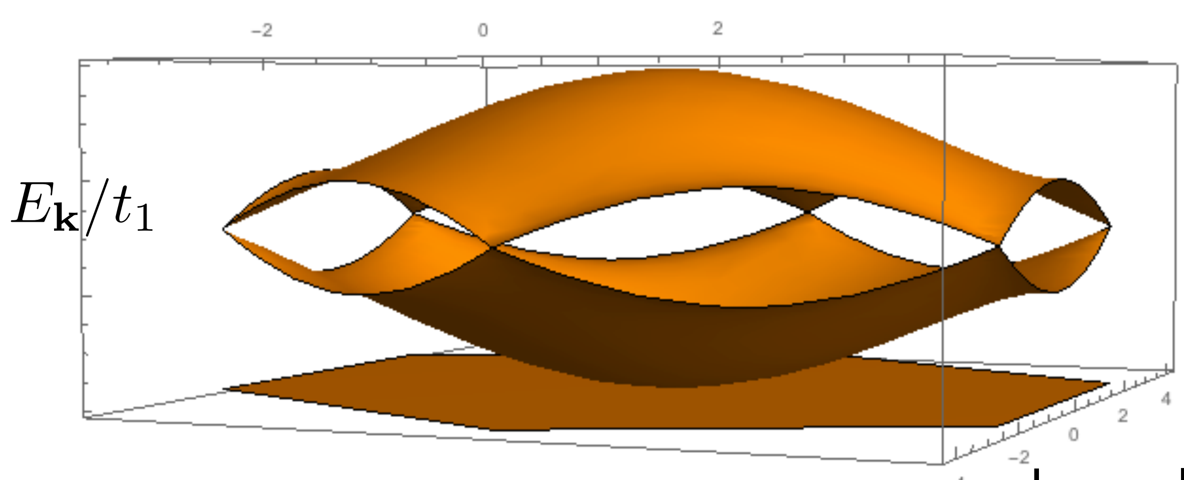
- Brief detour: localized modes on frustrated lattices
- Flat bands are easy to find in geometrically frustrated lattice models

  - Example: nearest neighbor hopping on a kagome lattice

$$H = t_1 \sum_{\langle i,j \rangle} c_i^\dagger c_j$$

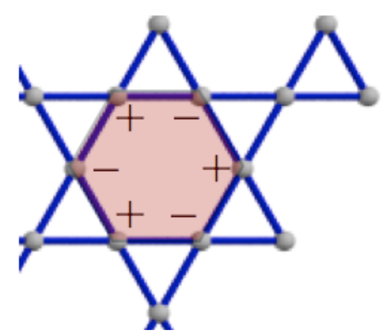
Bloch Hamiltonian: $$\mathcal{H}_{\mathbf{k}} = t_1 \begin{pmatrix} 0 & 1+e^{ik_1} & 1+e^{ik_2} \\ 1+e^{-ik_1} & 0 & 1+e^{-ik_3} \\ 1+e^{-ik_2} & 1+e^{ik_3} & 0 \end{pmatrix}$$





"Graphene + a flat band"

Localized modes explain the flat band



(but these are topologically trivial, and not Wannier functions!)

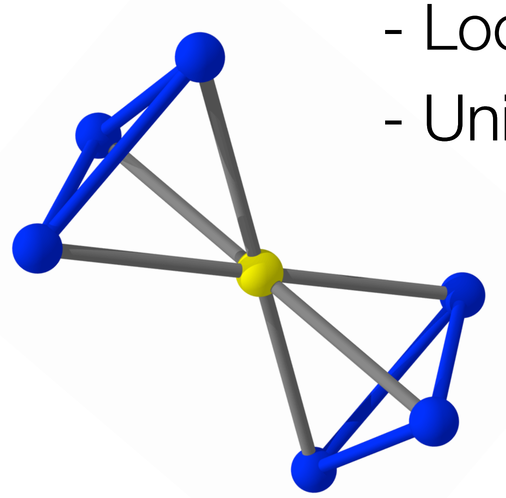
- Provides the connection we want -- and qualitatively new physics on the way!

Surface states

M. Trescher and E.J. Bergholtz, Phys. Rev. B 86, 241111(R) (2012)

E.J. Bergholtz, Z. Liu, M. Trescher, R. Moessner, and M. Udagawa, arXiv:1408.3669

- Despite the non-locality of the Wannier functions, geometrical frustration provides an avenue to novel surface states
- Crucial insight: surface bands localized to the kagome layers only if the total hopping amplitude to the triangular layer vanish.

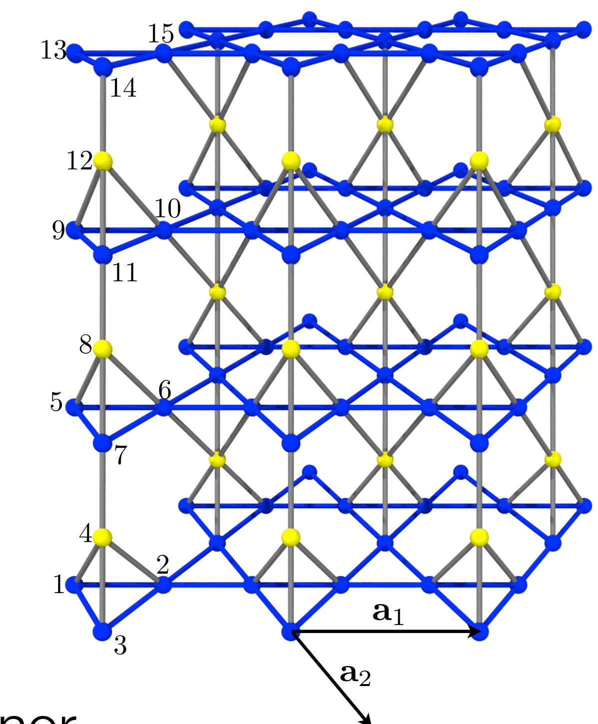


- Local constraint, destructive interference
- Unique solution, independent of details!

$$|\psi^i(\mathbf{k})\rangle = \mathcal{N}(\mathbf{k}) \sum_{m=1}^{N} \Big(r(\mathbf{k})\Big)^m |\phi^i(\mathbf{k})\rangle_m$$

$$r(\mathbf{k}) = -\frac{\phi_1^i(\mathbf{k}) + \phi_2^i(\mathbf{k}) + \phi_3^i(\mathbf{k})}{e^{-ik_2}\phi_1^i(\mathbf{k}) + e^{i(k_1-k_2)}\phi_2^i(\mathbf{k}) + \phi_3^i(\mathbf{k})}$$

components of the single layer Bloch spinor



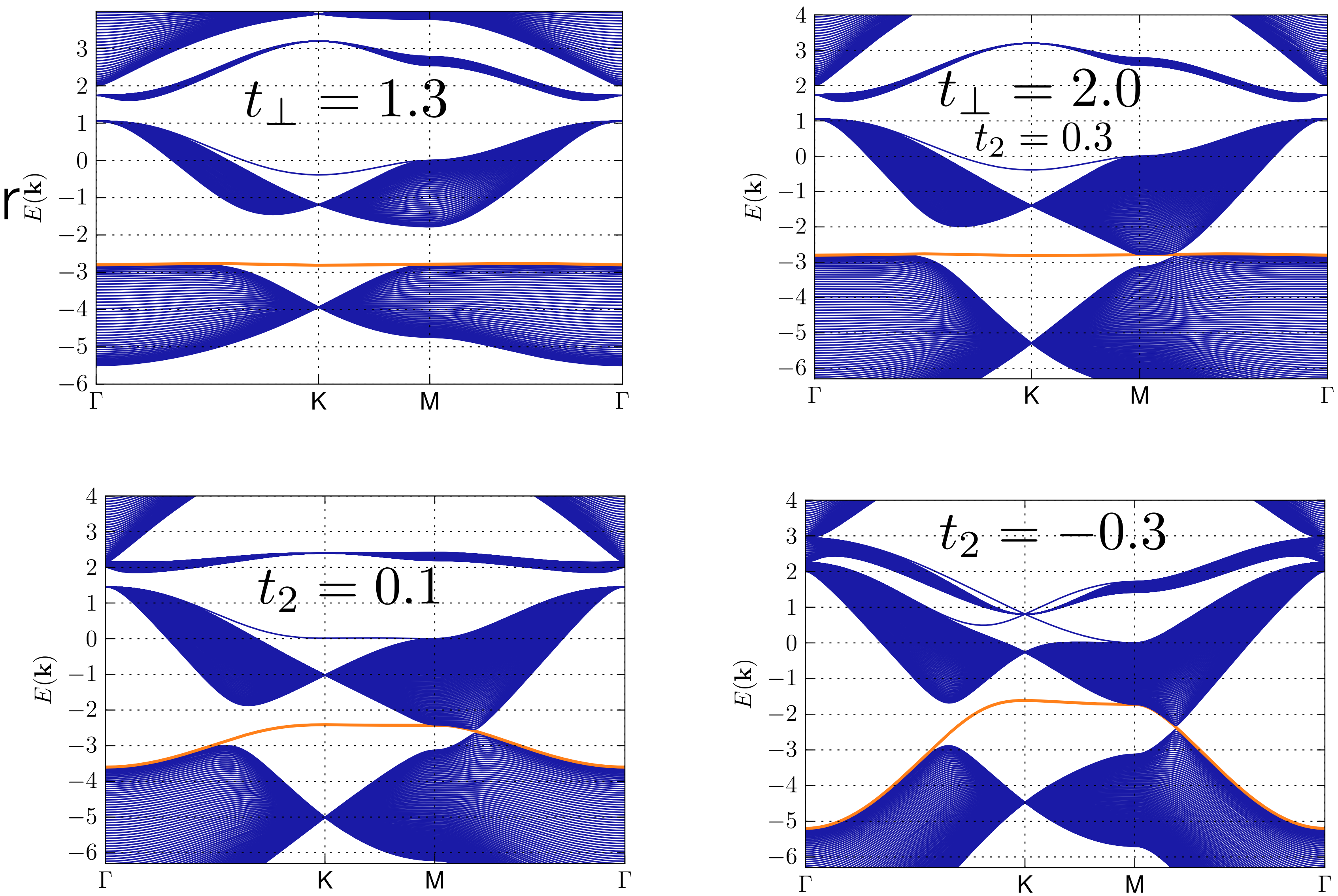
- Inherits the dispersion of the single layer model
- Localized to top or bottom layer, depending on $|r(\mathbf{k})|$

- When each kagome layer is a Chern insulator, these are precisely the states with Chern number C=N !
  - Simple way of generating (flat) bands with any Chern number

What's the nature of the surface states?

E.J. Bergholtz, Z. Liu, M. Trescher, R. Moessner, and M. Udagawa, arXiv:1408.3669

- Another look at the bulk spectrum...
- Increase the interlayer tunneling -- this leaves the flat band unchanged



- Change the nearest neighbor hopping
- Band touching described by the Weyl Hamiltonian

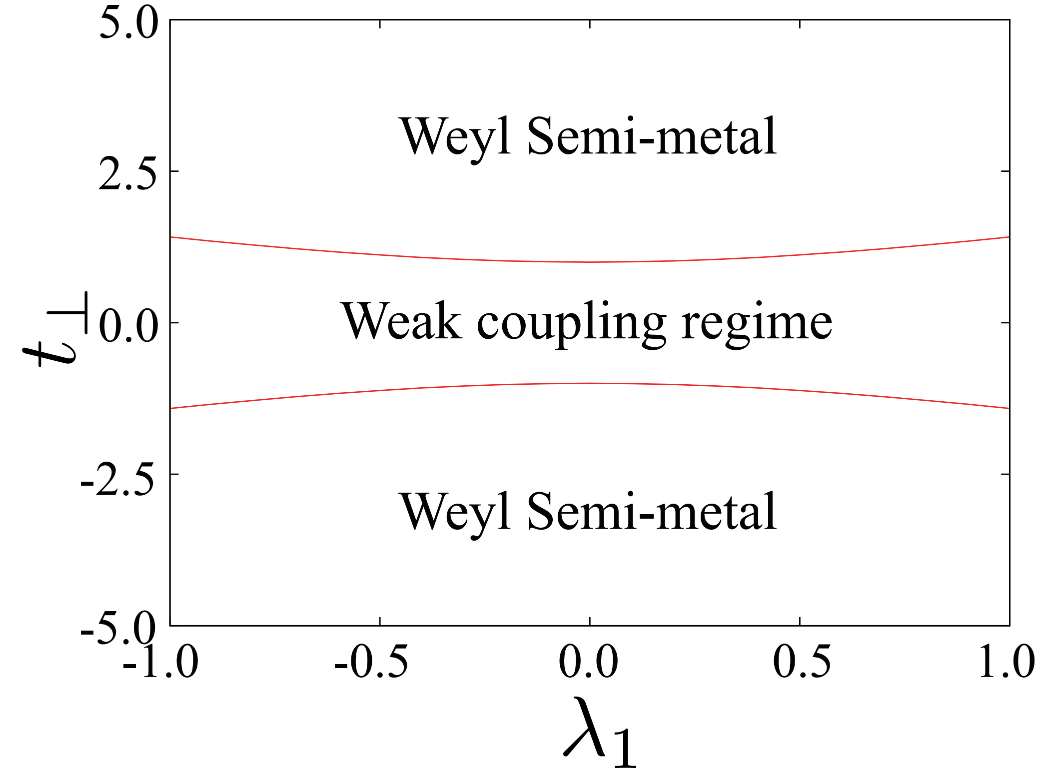
$$H_{\mathrm{Weyl}} = \sum_i v_i \sigma_i k_i + E_0(\mathbf{k})\mathbb{I}$$

- Nb. this holds in each case, also when the touching cone is nearly flat!

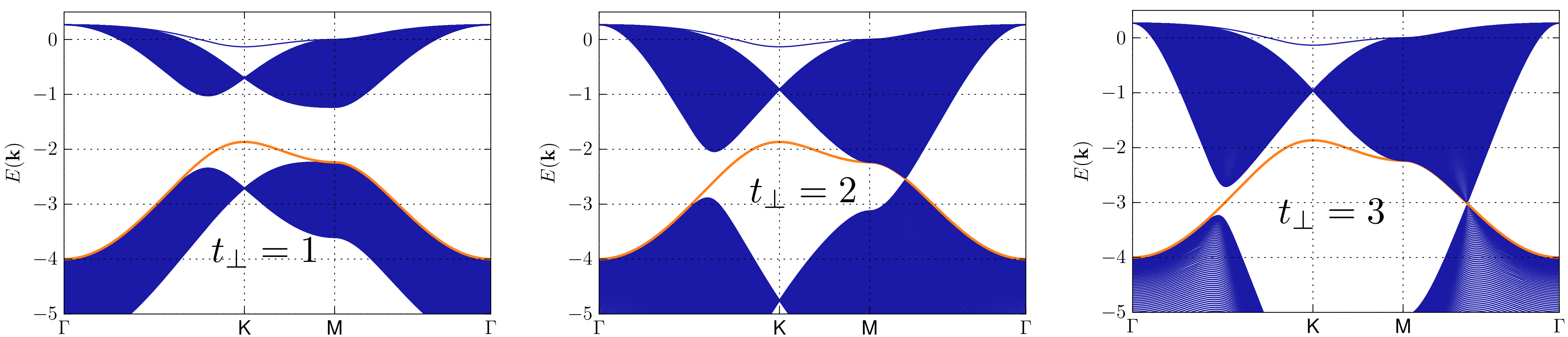
Works generically

E.J. Bergholtz, Z. Liu, M. Trescher, R. Moessner, and M. Udagawa, arXiv:1408.3669

- Phase diagram (more complicated for very strong spin-orbit coupling)



- Generic example $(t_1 = -1, \lambda_1 = 0.5)$



- Nb. the surface states are entirely independent on $t_\perp$

Weyl semi-metals

- Topological gapless phase in three dimensions

  - stable touching points, protected by a Chern number

  - Half a gapless Dirac theory

$$H_{\mathrm{Weyl}} = \sum_i v_i \sigma_i k_i + E_0(\mathbf{k})\mathbb{I}$$

  - many fascinating transport phenomena, e.g., the chiral anomaly

Reviews:

A.M. Turner and A. Vishwanath, Beyond Band Insulators: Topology of Semi-metals and Interacting Phases, arXiv:1301.0330

P. Hosur and X. Qi, Recent developments in transport phenomena in Weyl semimetals, arXiv:1309:4464

- Subject to intense experimental (and theoretical) activity

  - no ideal realization yet, but similar “Dirac metals” with symmetry protected Weyl features found recently

  - many new ideas and and engineered structures materials are being tested...

- Predicted in pyrochlore iridates

- Alternative layer prescription for WSMs exist

  - details and ingredients are however very different

X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Phys. Rev. B 83, 205101 (2011).

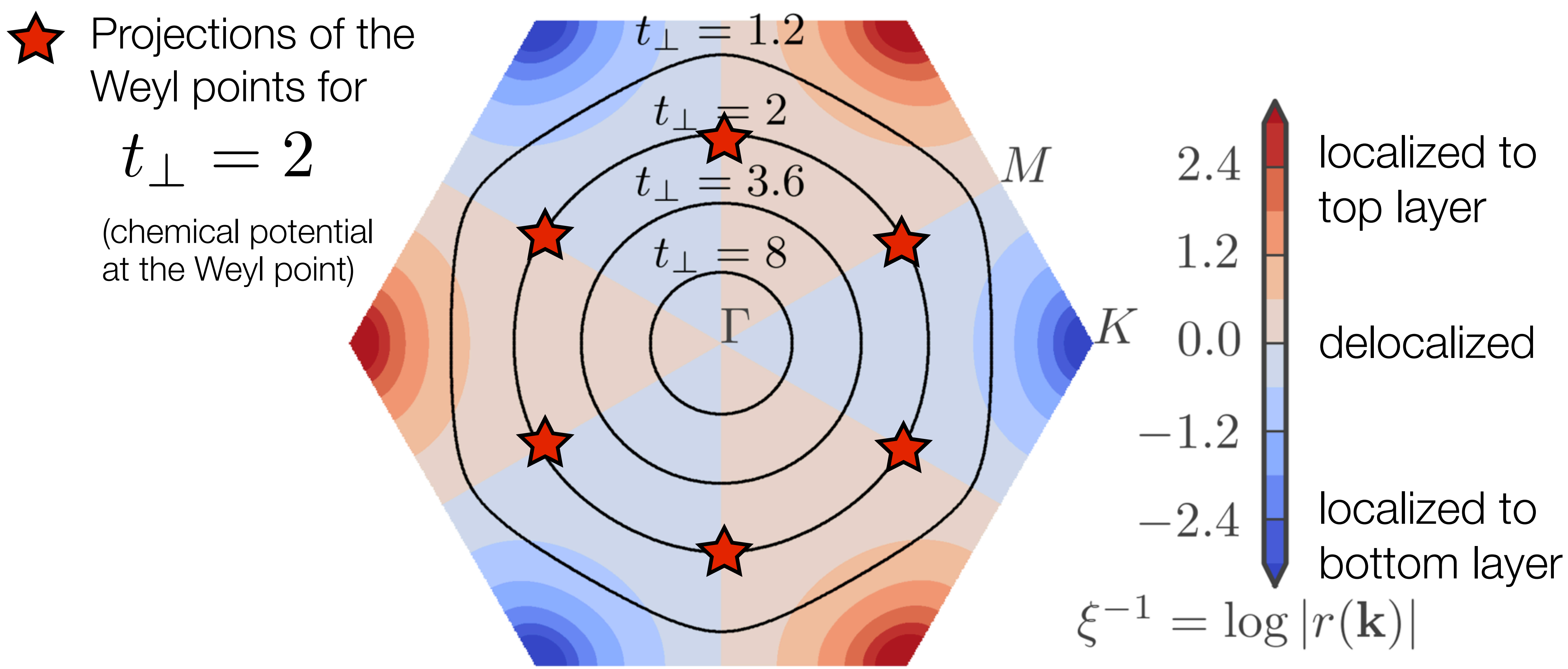
A. A. Burkov and L. Balents,, Phys. Rev. Lett. 107, 127205 (2011).

- The topology is manifested through exotic surface states, “Fermi arcs”

Fermi arcs in the pyrochlore slab

E.J. Bergholtz, Z. Liu, M. Trescher, R. Moessner, and M. Udagawa, arXiv:1408.3669

- Constant energy lines, “Fermi circles”, are split into Fermi arcs!



- Here we have an exact solutions for the Fermi arcs, and seen as a family, they carry a huge Chern number.
- The Fermi arcs also exist in absence of Weyl nodes in the bulk!

Summing up...

- Topology puts fundamental restrictions on locality.

  - Search algorithm for “sweet spots” (e.g. Kitaev chain)

  - Alternative approach to classify band topology

  - Wide range of potential applicability -- from first principles calculations to dissipative engineering etc.

- Local constraints are nevertheless useful for understanding and “engineering” new topological states of matter.

  - Novel FCIs in the Fermi arc surface bands of (thin) Weyl semi-metal slabs!

  - Generic scheme to use geometric frustration when engineering topological states

Useful to think about topological states in real-space

Thanks to my collaborators

Jan Carl Budich, Innsbruck
Sebastian Diehl, Innsbruck
Jens Eisert, Berlin
Peter Zoller, Innsbruck

Budich, et. al., arXiv:1405.6641

Zhao Liu, Princeton
Roderich Moessner, Dresden
Maximilian Trescher, Berlin
Masafumi Udagawa, Tokyo

Bergholtz, et. al., arXiv:1408.3669

and (on related projects)

Jörg Behrmann (Berlin), Piet Brouwer (Berlin), Eliot Kapit (Oxford), Heng Fan (Beijing), Dmitry Kovrizhin (Cambridge), Andreas Läuchli (Innsbruck), Samuel Sanchez (Berlin/ Copenhagen), Björn Sbierski (Berlin)

and thank you!

Related review: **Topological Flat Band Models and Fractional Chern Insulators**
E.J. Bergholtz and Z. Liu, *Int. J. Mod. Phys. B 27, 1330017 (2013)* [arXiv:1308.0343].