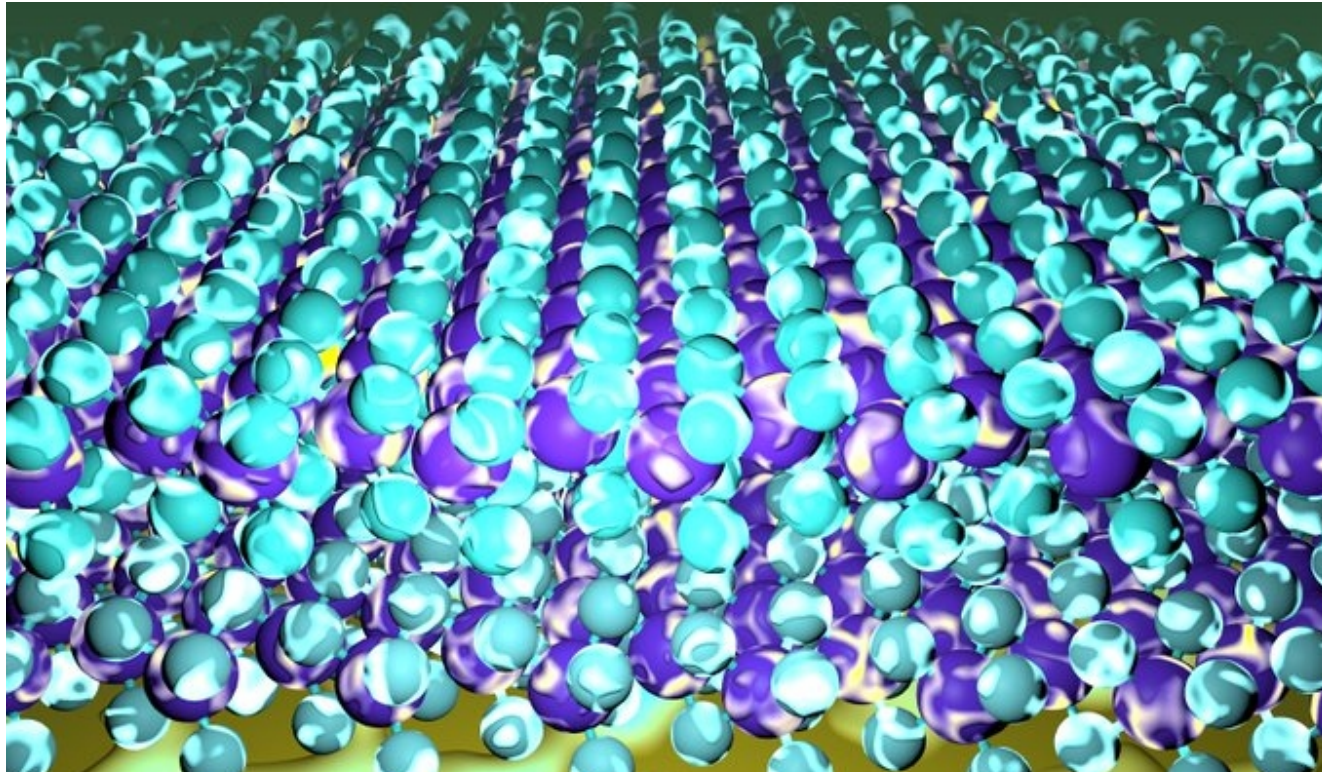




Topological states in van der Waals materials



Jyväskylä Summer School "Emergent Quantum Matter in Artificial Two-dimensional Materials"

Friday August 12th 2022

Schedule for the lecture

- 40 min lecture
- 15 min break
- 40 min lecture
- 15 min break
- 40 min lecture

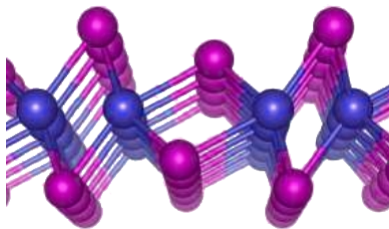


Today's plan

- The quantum Hall effect in 2D materials
- Van der Waals Chern insulators
- Van der Waals quantum spin Hall insulators
- Van der Waals quantum valley Hall insulators
- Topological phase transitions

Topological van der Waals materials

Quantum spin Hall insulators

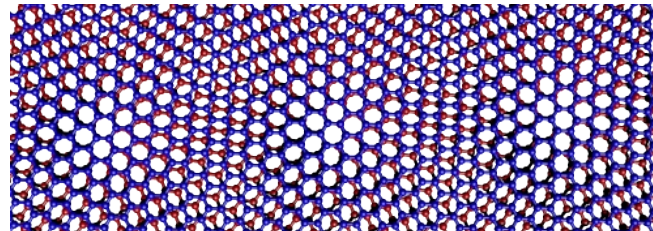


$1T'-WTe_2$

QH graphene

*Preserve
time-reversal
symmetry/ S_z*

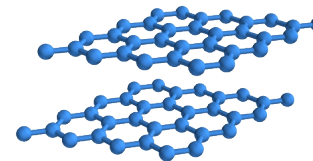
Chern insulators



Twisted graphene multilayers

*Break time-reversal
symmetry*

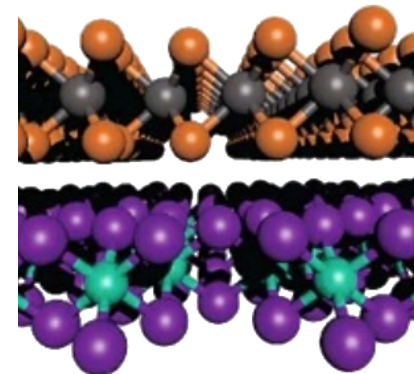
Valley Chern insulators



Bilayer
graphene

*Preserve valley
symmetry*

Topological superconductors



$CrBr_3/NbSe_2$

*Break gauge
symmetry*

Topology in electronic systems



Topological invariant in a Hamiltonian

We can classify Hamiltonians according to topological invariants

Hamiltonian

$$H(\mathbf{k})$$

Wavefunction

$$|\Psi(\mathbf{k})\rangle$$

$$C = \int_{BZ} \Omega d^2\mathbf{k}$$

**Topological invariant
(Chern number)**

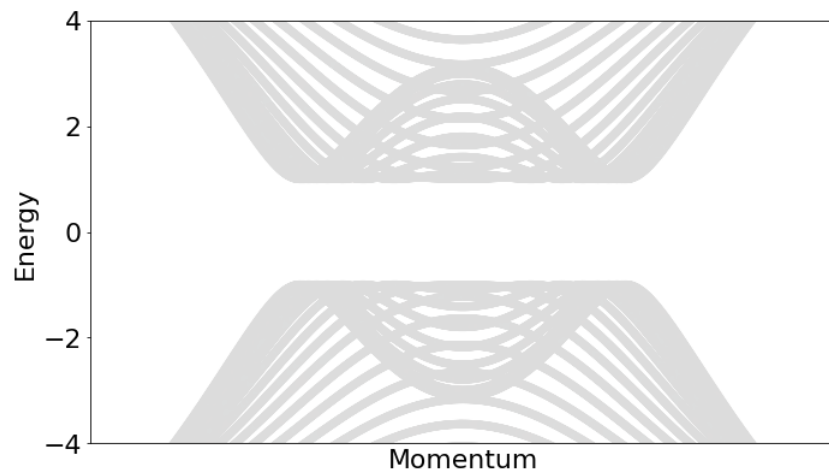
$$\Omega = \nabla \times \mathbf{A}|_z$$

**Metric
(Berry curvature)**

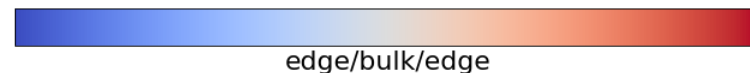
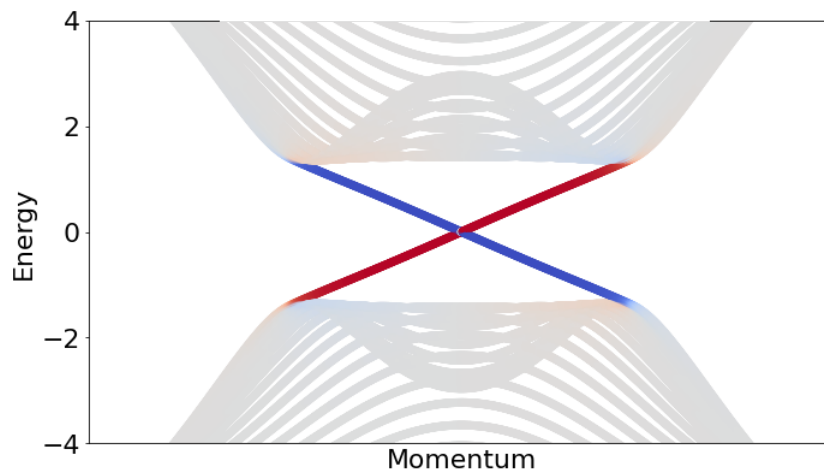
The role of a topological invariant

**Hamiltonians with different topological invariants
can not be deformed one to another without closing the gap**

$$C = 0$$

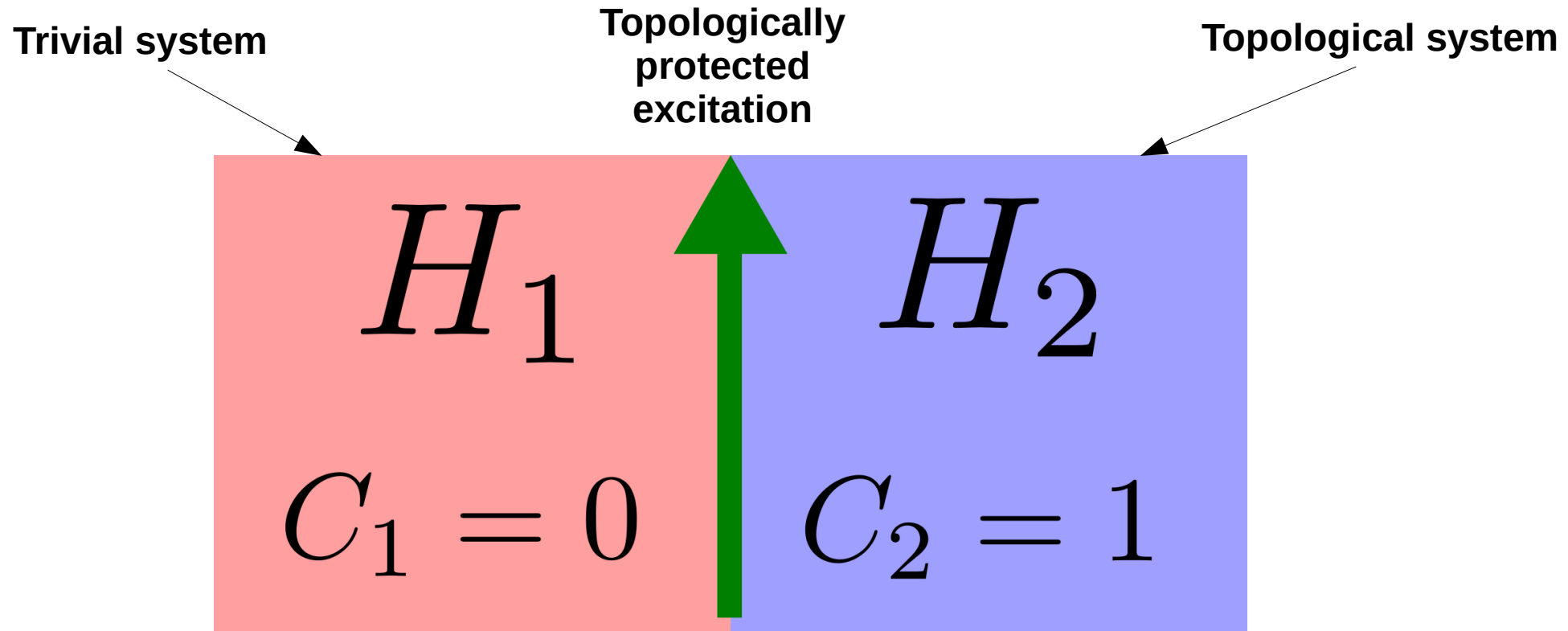


$$C = 1$$





The consequence of different topological invariants



Topological excitations appear between topologically different systems

The edge states of the quantum Hall effect

Trivial system

Topologically
protected
chiral state

Topological system

$$C_1 = 0$$

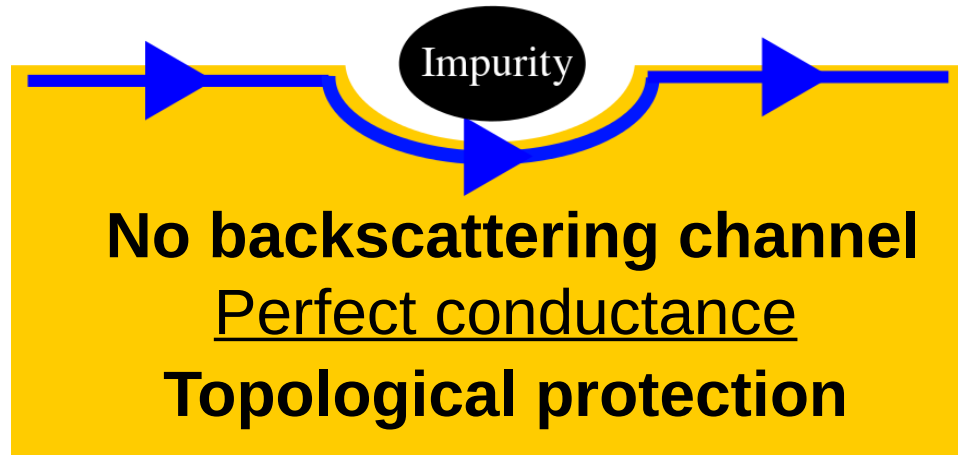


$$C_2 = 1$$

The edge states of the quantum Hall effect are topological excitations



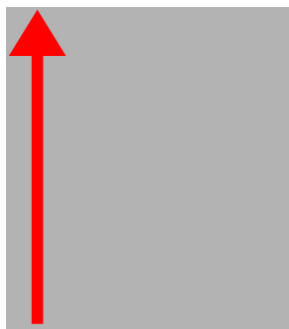
The edge states of the quantum Hall effect



The edge states of the quantum Hall effect are topologically protected

Four topological states in 2D materials

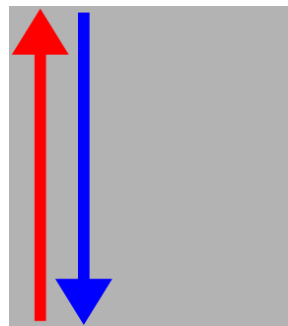
Chern insulators



Chiral states
Electronics

Twisted graphene
bilayer

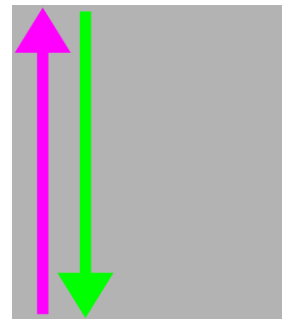
**Quantum spin
Hall insulators**



Helical states
Spintronics

1T'-WSe₂

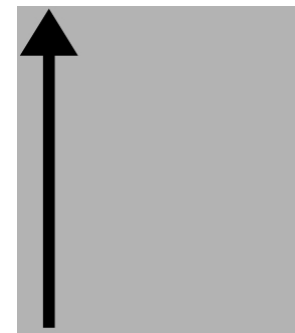
**Quantum valley
Hall insulators**



Valley-helical states
Valleytronics

Bilayer graphene

**Topological
superconductors**



Majorana excitations
*Topological quantum
computing*

CrBr₃/NbSe₂

Four topological states in 2D materials

Chern insulators

**Quantum spin
Hall insulators**

**Quantum valley
Hall insulators**

**Topological
superconductors**

$$C = 0, 1, 2, \dots$$

$$Z_2 = 0, 1$$

$$C_V = 0, 1, 2, \dots$$

$$C = 0, 1, 2, \dots$$

Chern number

Z_2 invariant

Valley Chern number

Chern number

Twisted graphene
bilayer

1T'-WSe₂

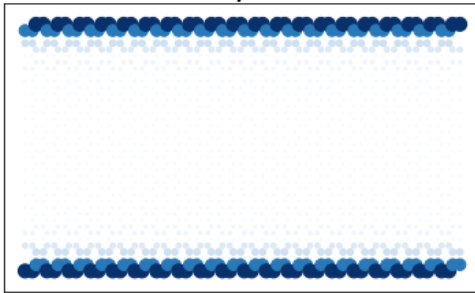
Bilayer graphene

CrBr₃/NbSe₂

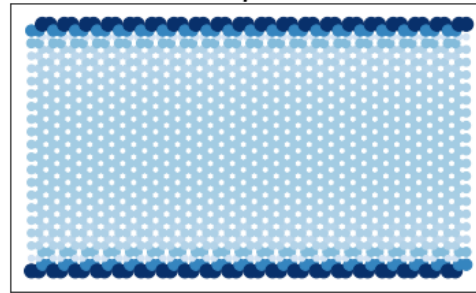
Location of states in a Chern insulator

States at zero energy for different chemical potentials in a Chern insulator

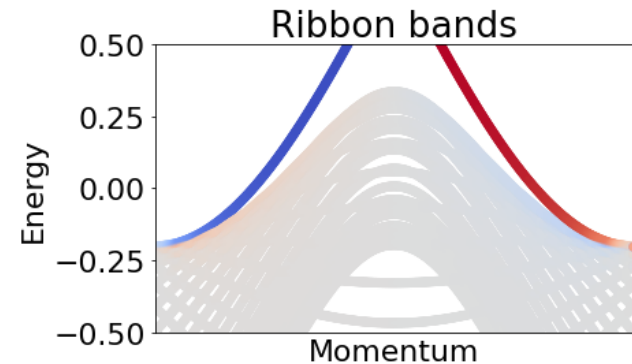
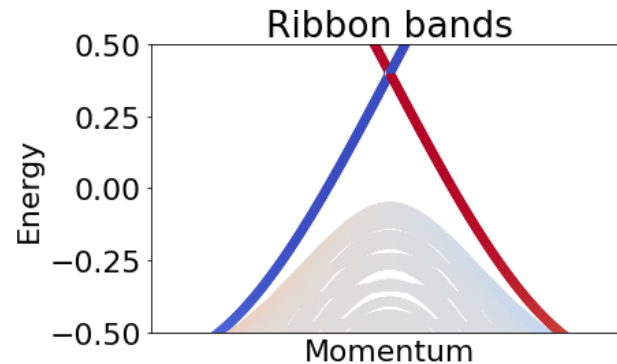
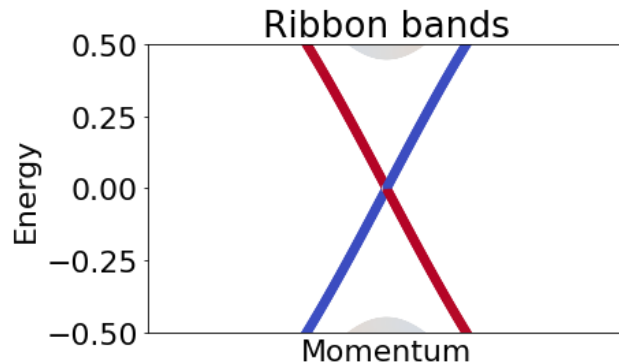
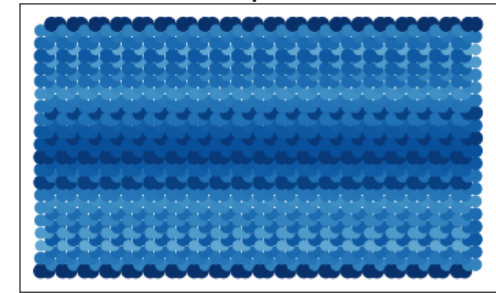
LDOS, $\mu = 0.0$



LDOS, $\mu = 0.4$



LDOS, $\mu = 0.8$

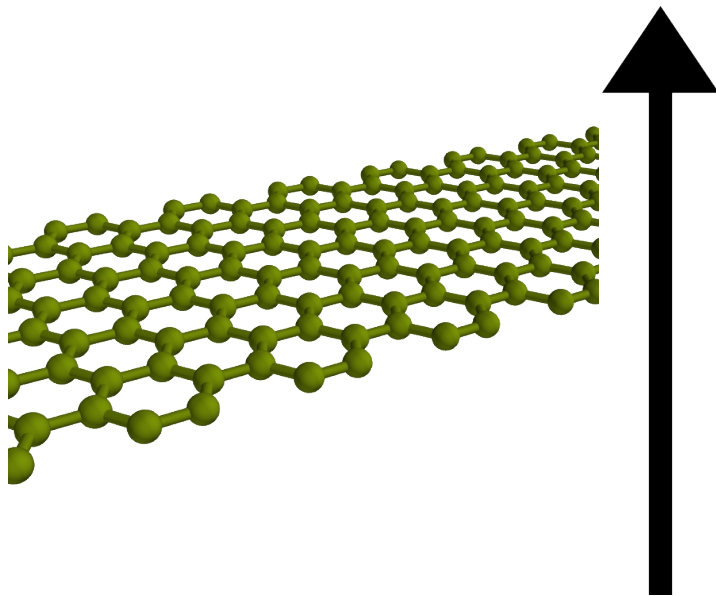


States in the gap are located at the edge, where above the gap states are located in the bulk

The quantum Hall effect

The quantum Hall effect

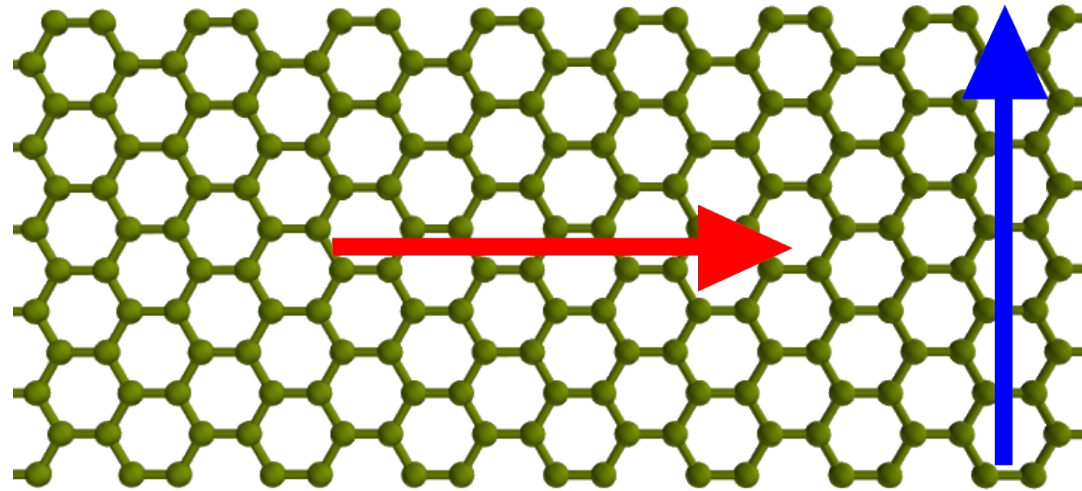
Take graphene in the presence of a very large magnetic field



Apply a magnetic field in z



Measure a current in x

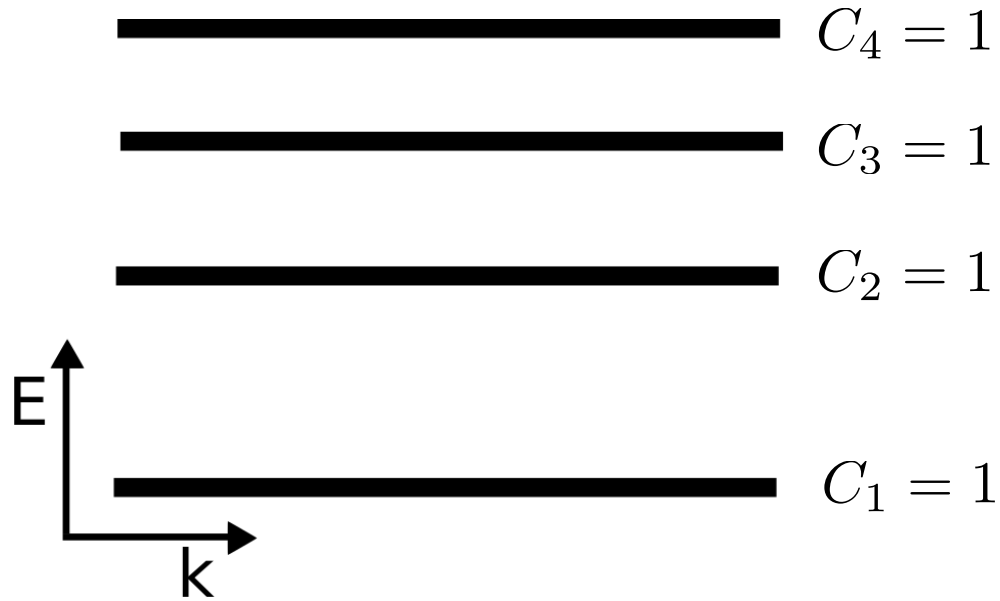


Apply a voltage in y

$$J_x = \sigma_{xy} V_y \quad \sigma_{xy} = 0, 1, 2, 3$$

The quantum Hall effect

Band-structure in the quantum Hall state



Hall conductivity

$$\sigma_{xy} = \sum_{\alpha \in occ} \int \Omega_{\alpha} d^2 \mathbf{k} = \sum_{\alpha} C_{\alpha} = C$$

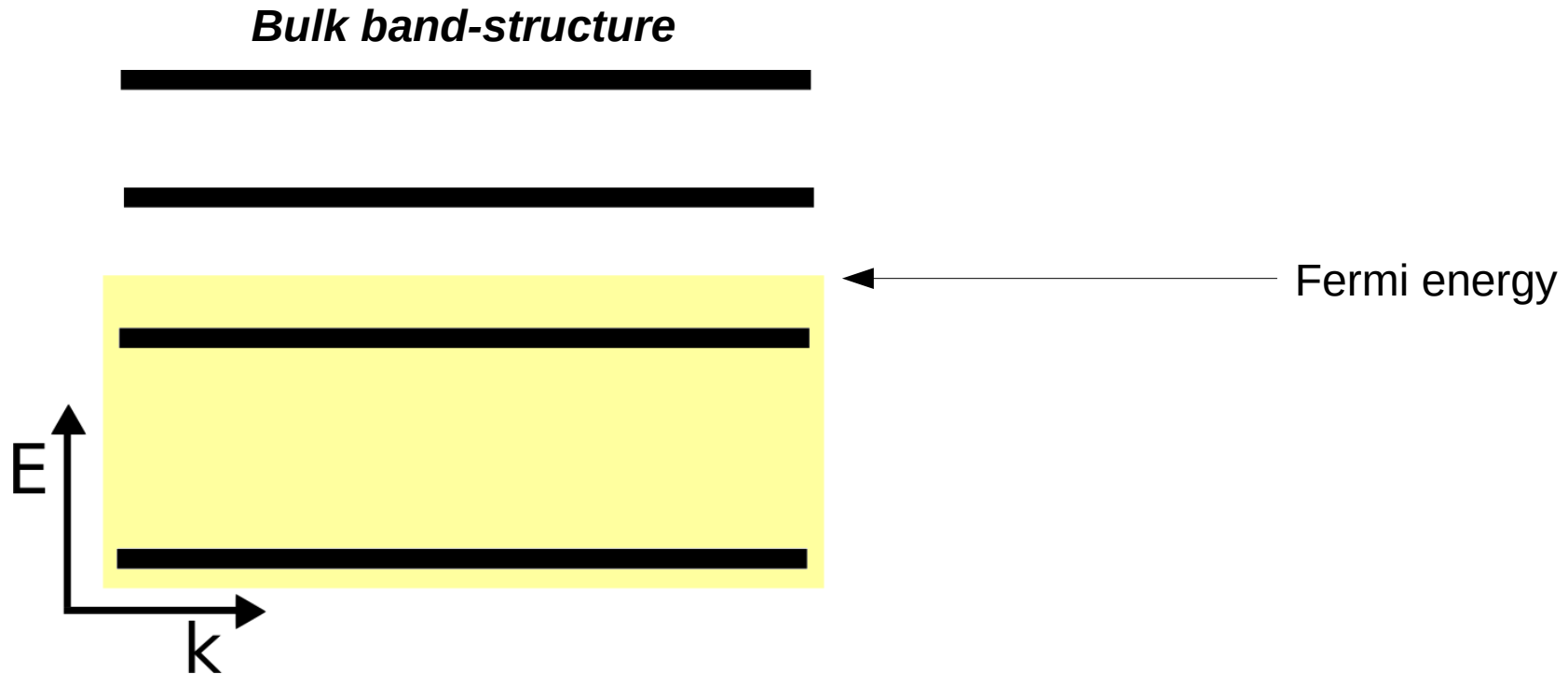
$$\Omega_{\alpha} = \partial_{k_x} A_y^{\alpha} - \partial_{k_y} A_x^{\alpha}$$

$$A_{\mu}^{\alpha} = i \langle \partial_{k_{\mu}} \Psi_{\alpha} | \Psi_{\alpha} \rangle$$

Each band (a.k.a Landau level), contributes with Chern number +1

The quantum Hall effect

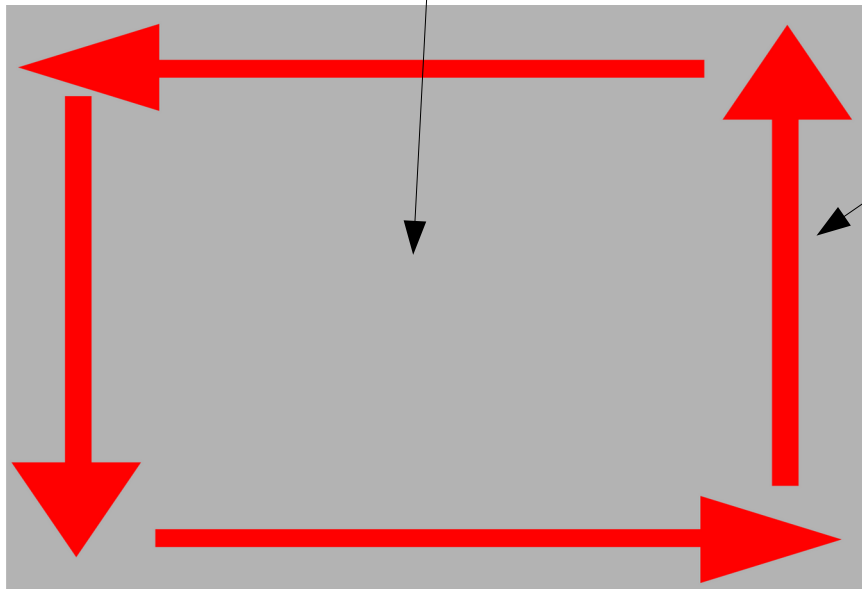
How can an insulator have conductivity?





The quantum Hall effect

The bulk of a quantum Hall state is insulating



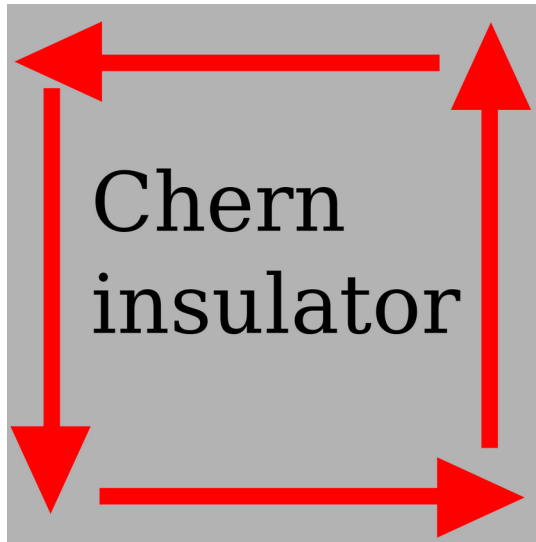
The edge has chiral states

Chiral: propagating only in one direction

Hall conductivity in an insulator

$$\sigma_{xy} = \sum_{\alpha \in occ} \int \Omega_{\alpha} d^2 \mathbf{k} = \sum_{\alpha} C_{\alpha} = C$$

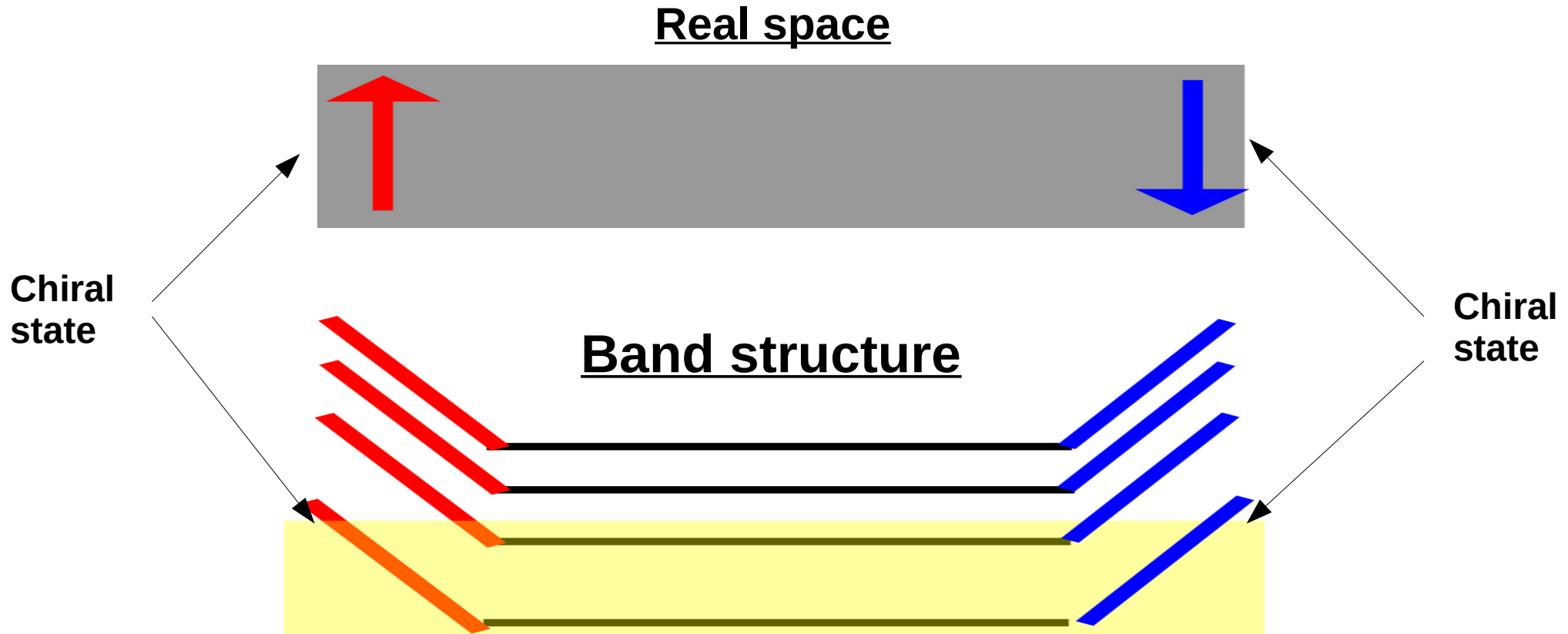
The Chern number for each band is quantized $C_{\alpha} = \int \Omega_{\alpha}(\mathbf{k}) d^2 \mathbf{k} = 0, \pm 1, \pm 2, \dots$



***An insulator can have a finite
(and quantized) Hall conductivity***

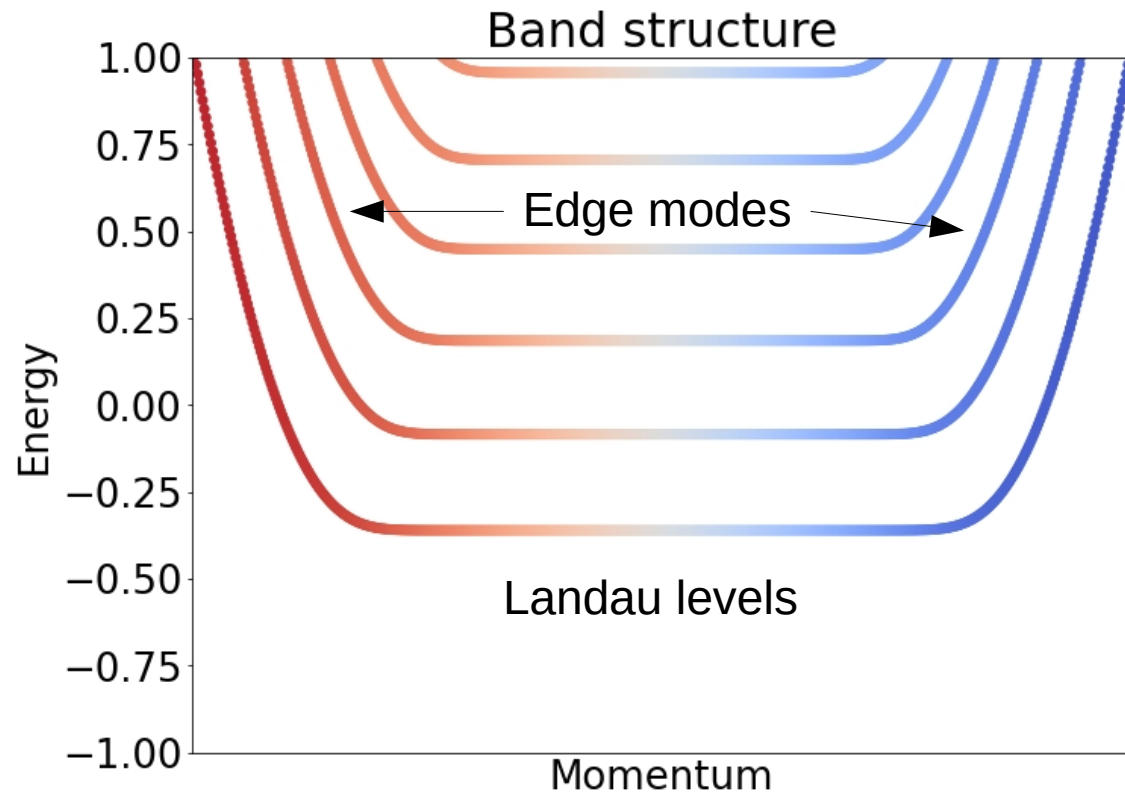
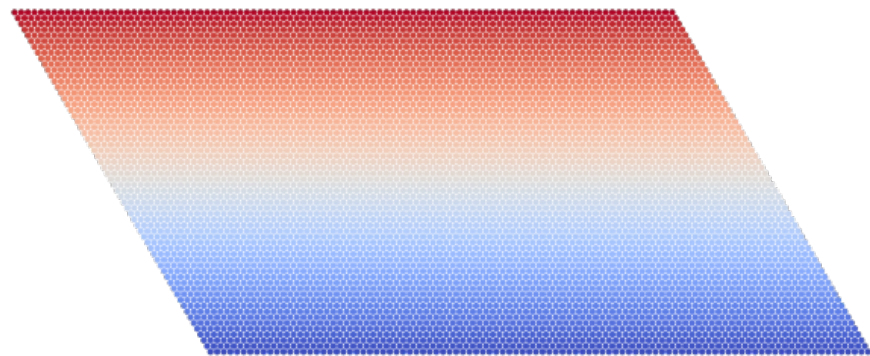
**This is a simple example of
a topological state of matter**

The quantum Hall effect



The quantum Hall effect in a 2D TMDC

Position operator



2D electrons in a magnetic field



Coupling electrons to a gauge field

The continuum limit

$$H = \frac{p^2}{2}$$

Given the kinetic energy without magnetic field

By replacing momentum by the canonical momentum
we recover the equations of motion in a magnetic field

$$H = \frac{\Pi^2}{2}$$

$$\Pi = \mathbf{p} + \mathbf{A}$$

Canonical momentum

$$\mathbf{B} = \nabla \times \mathbf{A}$$

Magnetic field

Magnetic vector potential

Coupling electrons to a gauge field

$$H = \frac{\Pi^2}{2}$$

$$\Pi = \mathbf{p} + \mathbf{A}$$

Canonical momentum

$$p_\alpha = -i\partial_\alpha$$

Quantized momentum

Hamiltonian for electrons in a magnetic field

$$H = \frac{(\sum_\alpha -i\partial_\alpha + A_\alpha)^2}{2}$$

$$\Psi(\mathbf{r})$$

Gauge #1

$$H = \frac{(\sum_\alpha -i\partial_\alpha)^2}{2}$$

$$e^{i \int_0^{\mathbf{r}} \mathbf{A}(\mathbf{r}') d\mathbf{r}'} \Psi(\mathbf{r})$$

Gauge #2

Coupling electrons to a magnetic field in a tight binding model

Given a tight-binding model without magnetic field

$$H = \sum t_{ij} c_i^\dagger c_j$$

Coupling to a magnetic field transforms the hoppings as

$$t_{ij} \rightarrow e^{i \int_{\mathbf{r}_i}^{\mathbf{r}_j} \mathbf{A}(\mathbf{r}') d\mathbf{r}'} t_{ij}$$

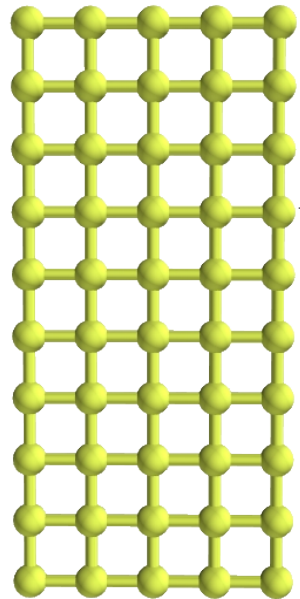
Leading (in the Landau gauge) to the Hamiltonian

$$H = \sum t_{ij} e^{iB(x_i - x_j)(y_i + y_j)} c_i^\dagger c_j$$

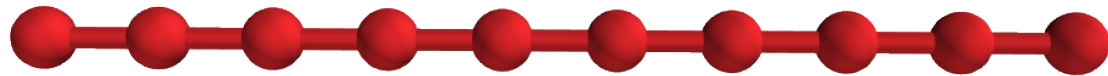
Quantum Hall effect and quasiperiodicity

Let us take the Hamiltonian in a magnetic field, and solve in a square ribbon

$$H = \sum t_{ij} e^{iB(x_i - x_j)(y_i + y_j)} c_i^\dagger c_j$$



Fourier transform in
the infinite direction

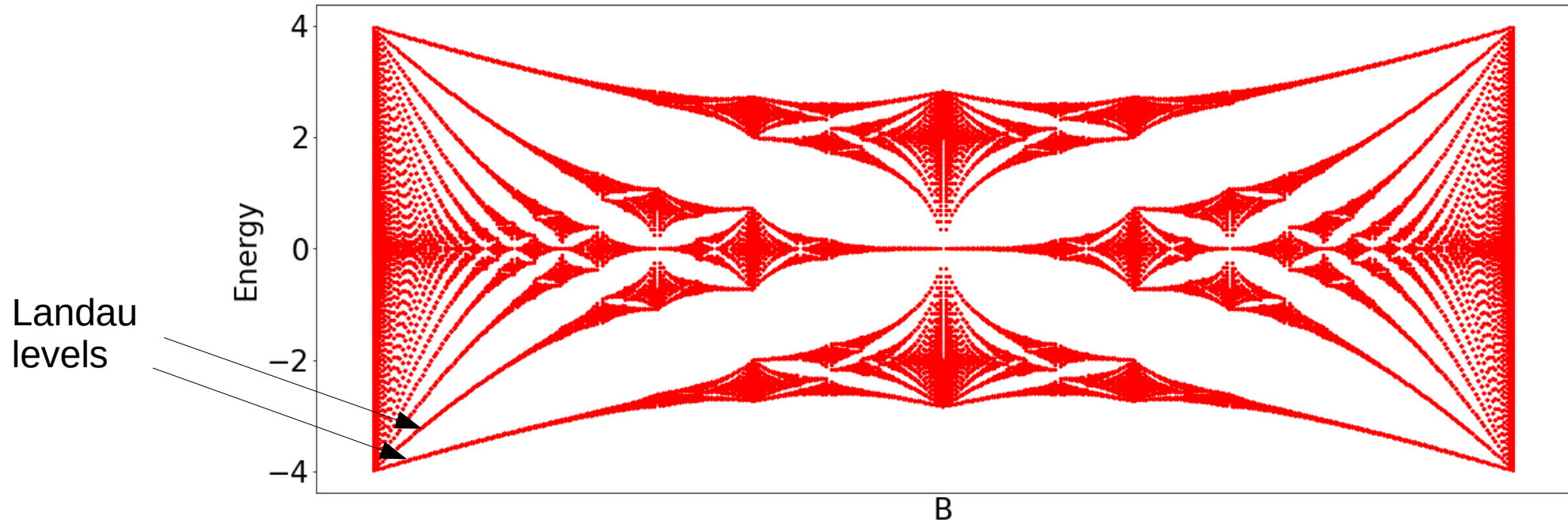


$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + 2 \sum_n \cos(Bn) c_n^\dagger c_n$$

The spectrum of 2D quantum Hall is the one of a 1D quasiperiodic moire

Quantum Hall effect and quasiperiodicity

$$H = \sum t_{ij} e^{iB(x_i - x_j)(y_i + y_j)} c_i^\dagger c_j$$



The spectrum of 2D quantum Hall is the one of a 1D quasiperiodic moiré

Two ways of coupling electrons to a magnetic field

Continuum limit

Schrodinger electrons $H = \frac{\Pi^2}{2}$

Dirac electrons $H = \sum_{\alpha} \Pi_{\alpha} \sigma_{\alpha}$

$$\Pi = \mathbf{p} + \mathbf{A}$$

Canonical momentum

Tight binding model

$$H = \sum t_{ij} c_i^{\dagger} c_j$$

$$t_{ij} \rightarrow e^{i\phi_{ij}} t_{ij}$$

$$\phi_{ij} = \int_{\mathbf{r}_i}^{\mathbf{r}_j} \mathbf{A}(\mathbf{r}') d\mathbf{r}'$$

Peierls substitution

For typical materials
 $\phi_{ij} \sim 10^{-4} \sim 10T$

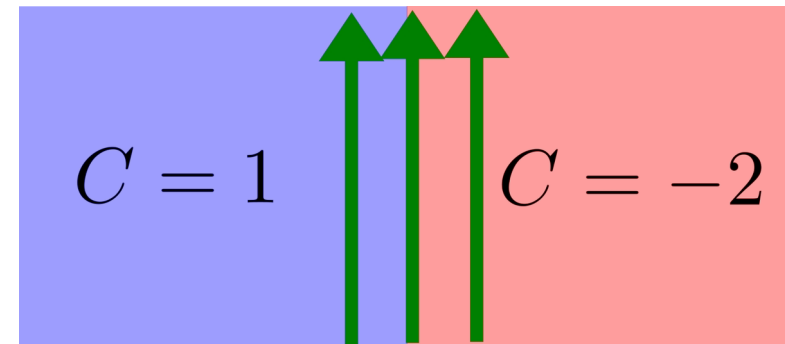
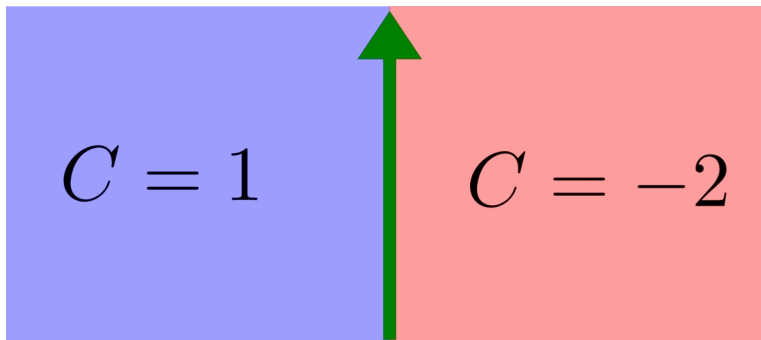


Break

10-15 min break

(optional) to discuss during the break

Given Chern numbers below, which image show the right number of edge states?



Landau levels

Landau levels

Band-structure in the quantum Hall state


$$n = 3$$

$$n = 2$$

$$n = 1$$

$$n = 0$$

The energy levels are

$$E \sim \left(n + \frac{1}{2} \right) B$$

$$E \sim 1 \text{ meV}$$

For a Dirac equation they would be

$$E \sim \sqrt{nB}$$

$$E \sim 50 \text{ meV}$$

The gauge of the magnetic potential

Let us consider the simplest magnetic field

$$\mathbf{B} = (0, 0, B_z)$$

We can write down two different gauges for the magnetic potential $\mathbf{B} = \nabla \times \mathbf{A}$

Landau gauge

$$\mathbf{A} = (-B_z y, 0, 0)$$

Respects one translational symmetry

$$[p_x, A_\alpha] = 0$$

Symmetric gauge

$$\mathbf{A} = \frac{1}{2}(-B_z y, B_z x, 0)$$

Convenient for the fractional quantum Hall wavefunction

Electrons coupled to a magnetic field

Let us take a conventional electron gas coupled to a gauge field

$$H = \frac{(\sum_{\alpha} -i\partial_{\alpha} + A_{\alpha})^2}{2}$$

Momentum

Gauge potential

Minimal gauge coupling

Landau levels of non-Dirac 2D materials

Lets take a quadratic Hamiltonian $H \sim p_x^2 + p_y^2$

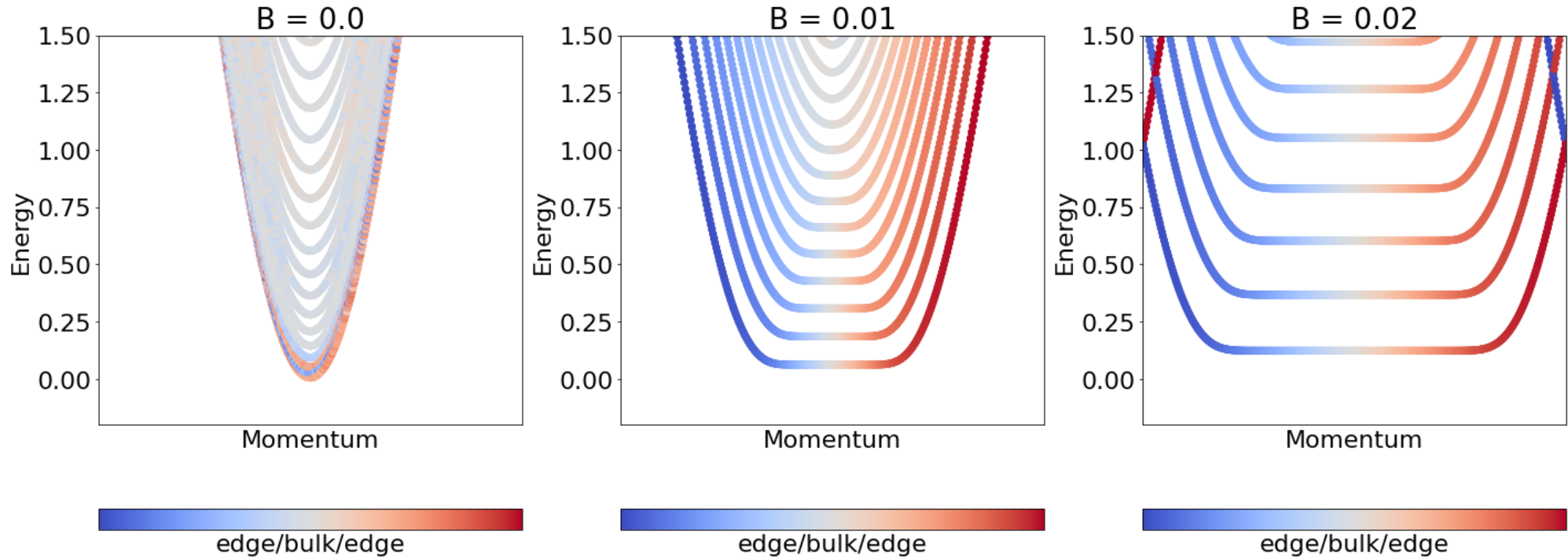
And add a magnetic field (minimal coupling) $\mathbf{p} \rightarrow \mathbf{p} + \mathbf{A}$

Take the Landau gauge $\mathbf{A} = (0, -Bx, 0)$
 $\nabla \times \mathbf{A} = (0, 0, B)$

Plugging the magnetic potential in we get $H \sim p_x^2 + B^2 x^2$
(this looks like an harmonic oscillator)

Quantized levels in a magnetic field $E_n \sim nB$

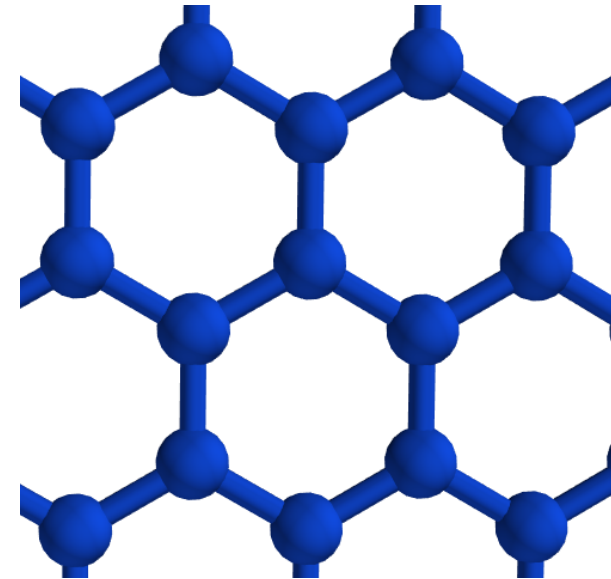
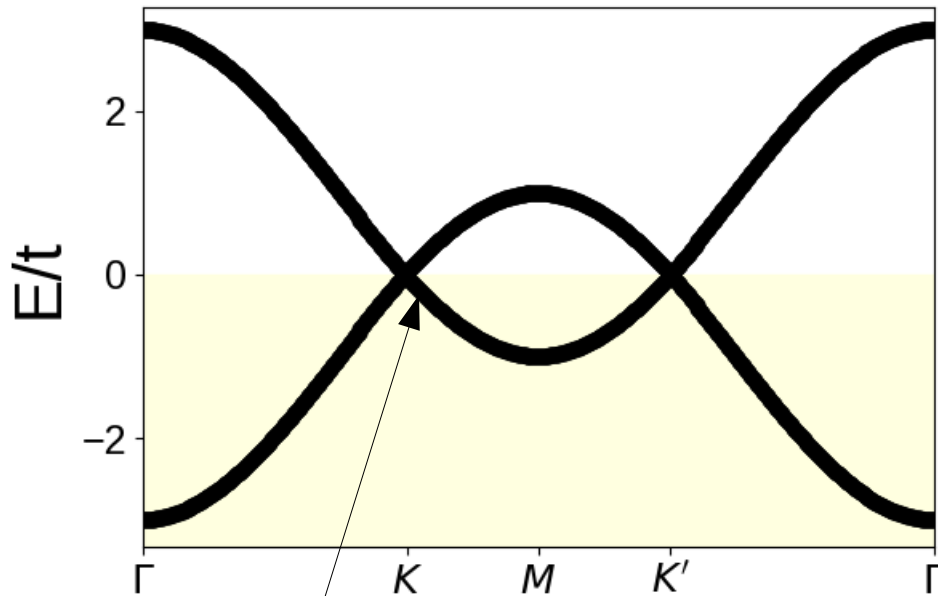
Landau levels of a 2D TMDC



As the magnetic field is increased, flat band Landau levels appear

The Landau levels of graphene

Band structure of a honeycomb lattice



Effective Dirac equations

Landau levels of graphene

Lets take a Dirac Hamiltonian

$$H \sim \begin{pmatrix} 0 & p_x + ip_y \\ p_x - ip_y & 0 \end{pmatrix}$$

And add a magnetic field (minimal coupling)

$$\mathbf{p} \rightarrow \mathbf{p} + \mathbf{A}$$

Take the Landau gauge

$$\mathbf{A} = (0, -Bx, 0)$$

$$\nabla \times \mathbf{A} = (0, 0, B)$$

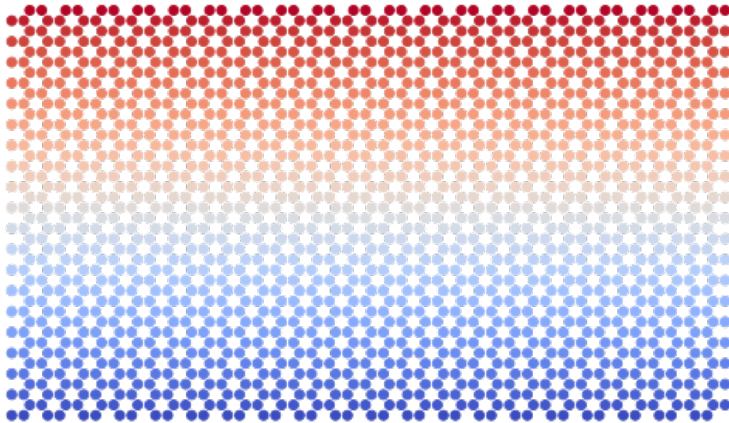
Plugging the magnetic potential in we get $H^2 \sim p_x^2 + B^2 x^2$

(this looks like an harmonic oscillator) $E_n^2 \sim nB$

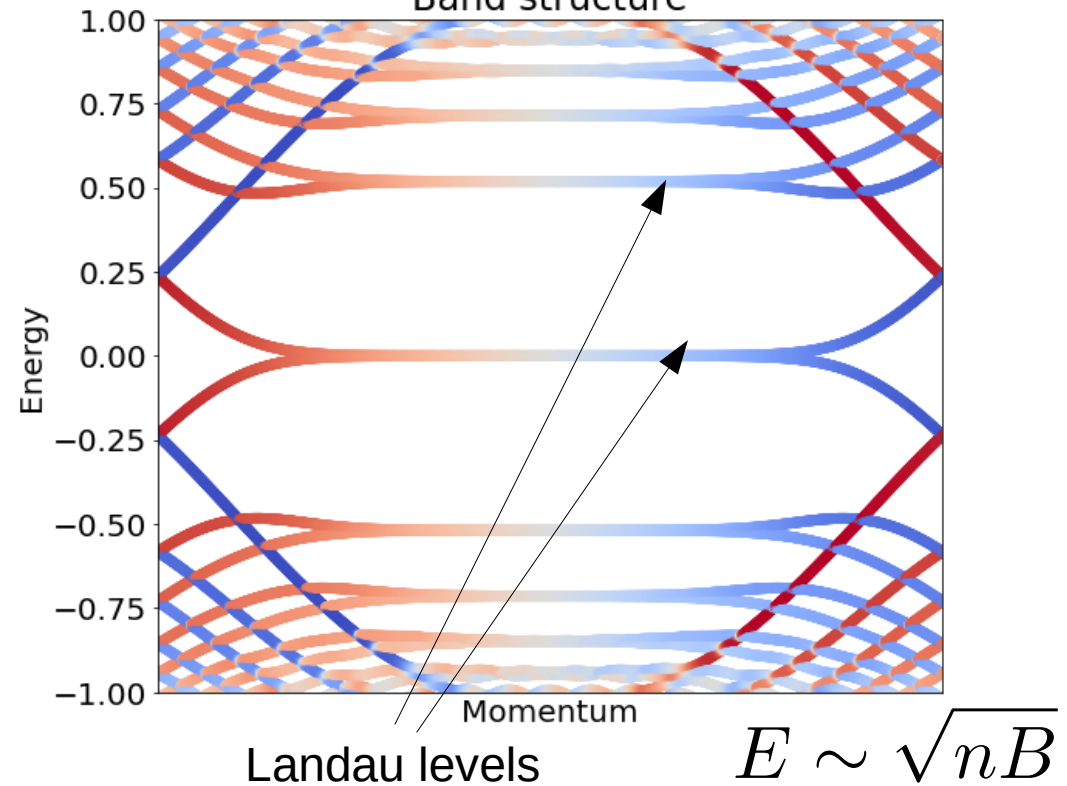
Quantized levels in a magnetic field $E_n \sim \sqrt{nB}$

The Landau levels in graphene

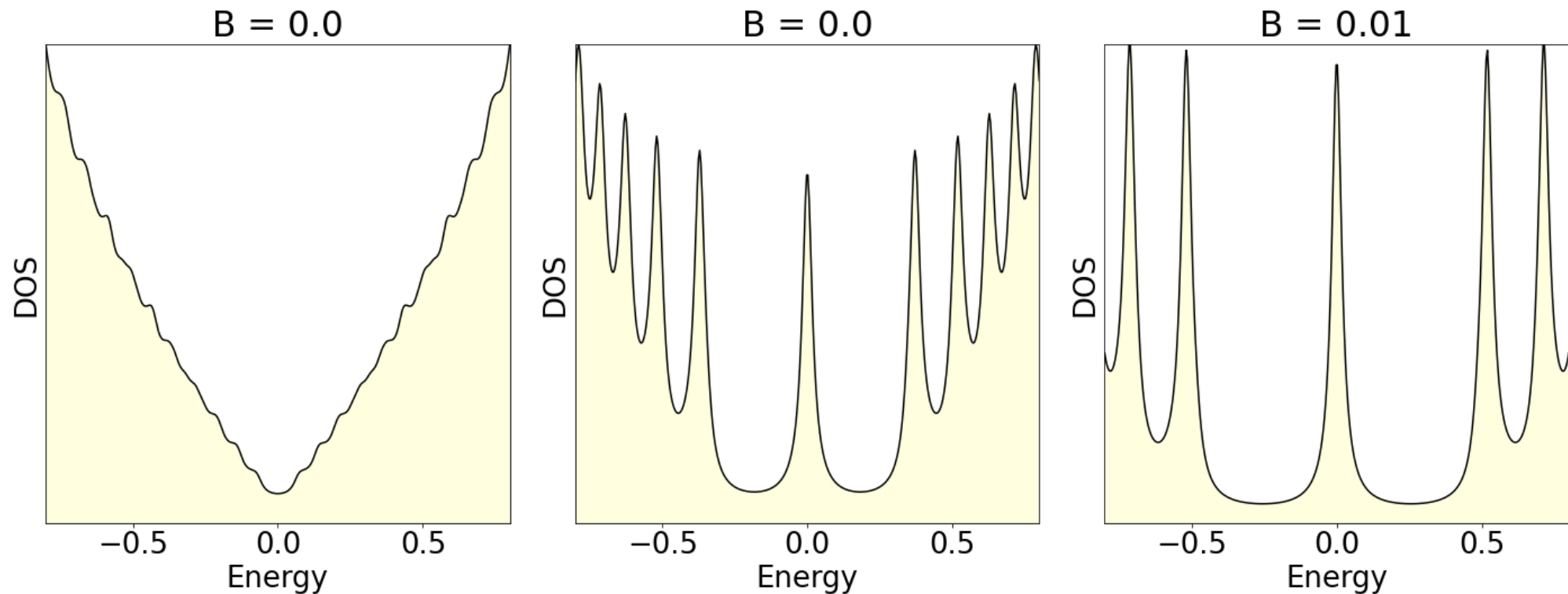
Position operator



Band structure

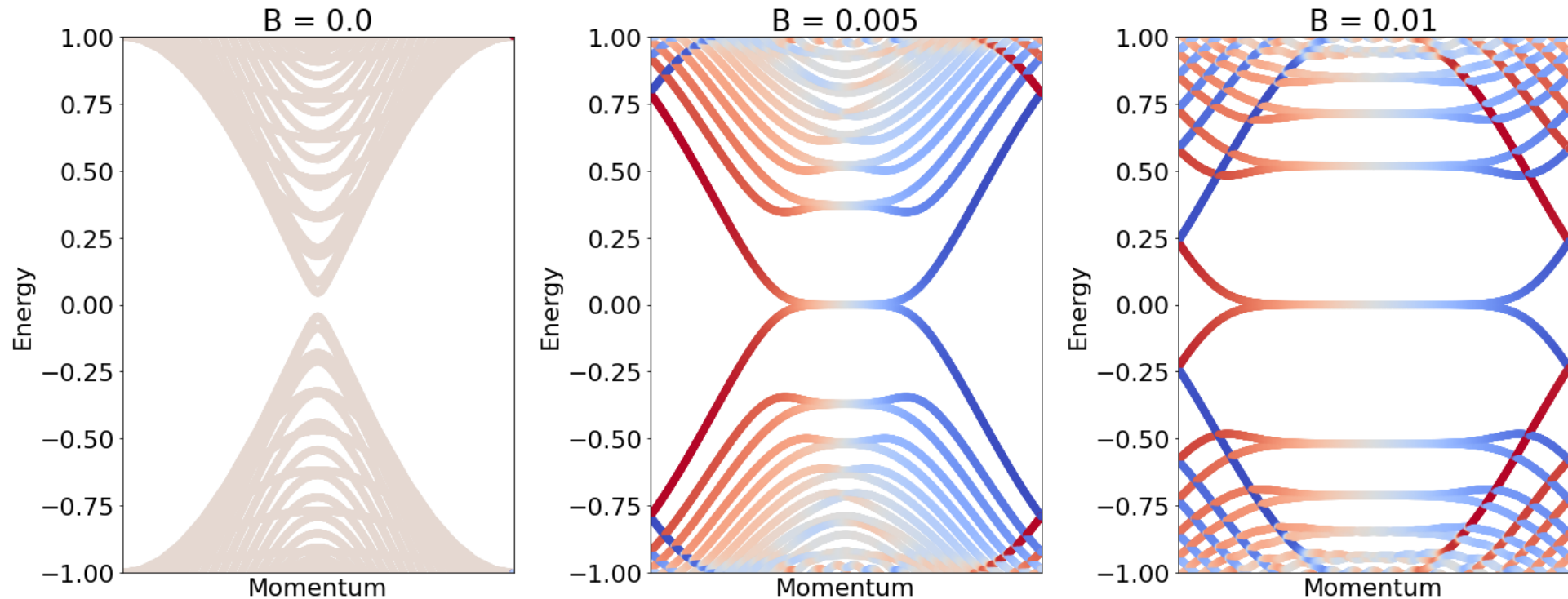


Graphene spectra in a magnetic field



A magnetic field largely enhances the DOS in graphene, allowing for instabilities to appear

The Landau levels in graphene



The zeroth Landau level in graphene

In the Dirac equation, each valley contributed with one Landau level at $E=0$

$$\Psi_K^{0LL} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \begin{array}{l} \text{Sublattice A} \\ \text{Sublattice B} \end{array}$$

$$\Psi_{K'}^{0LL} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \begin{array}{l} \text{Sublattice A} \\ \text{Sublattice B} \end{array}$$

In the absence of symmetry breaking

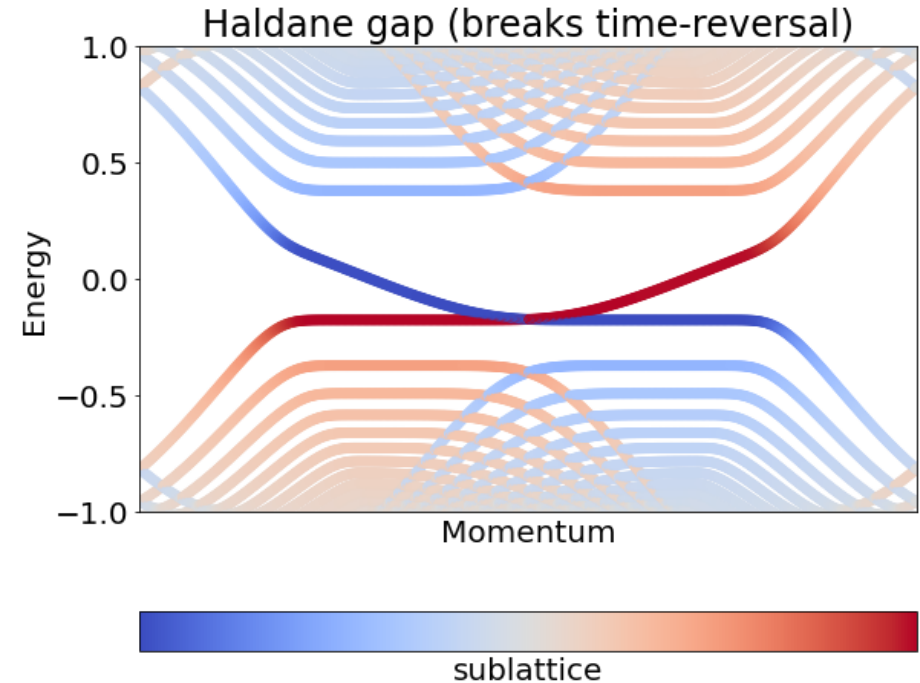
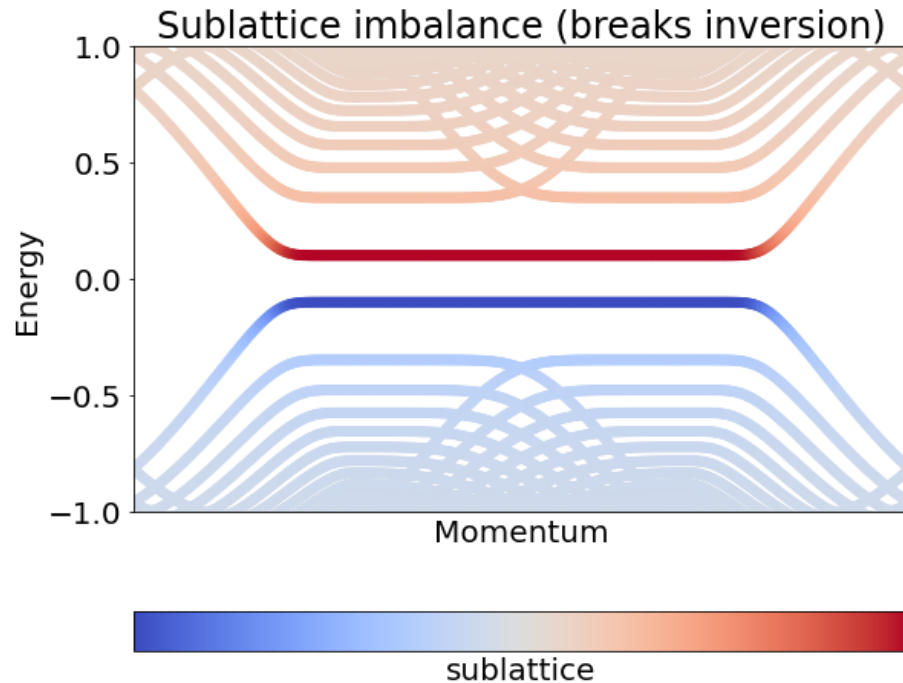


In the presence of symmetry breaking



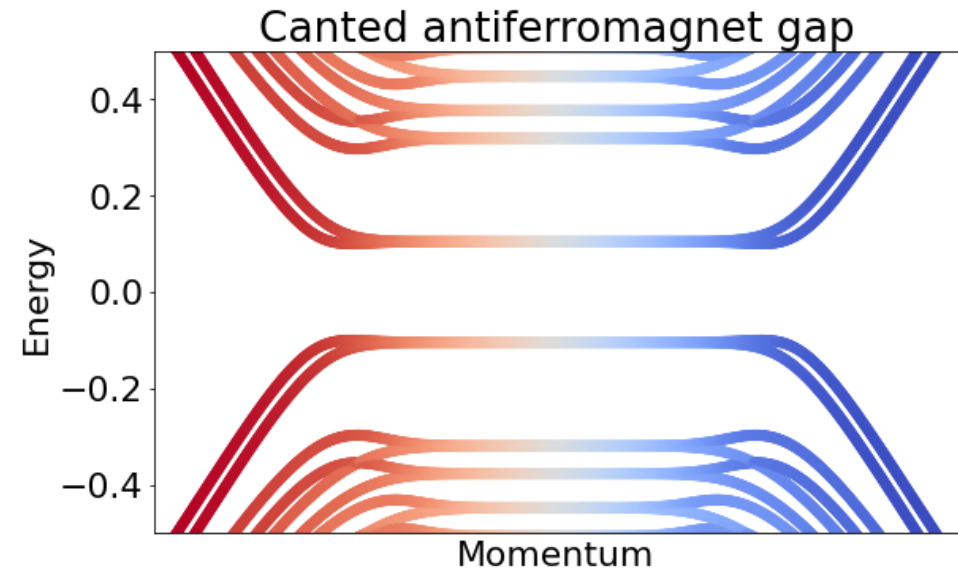
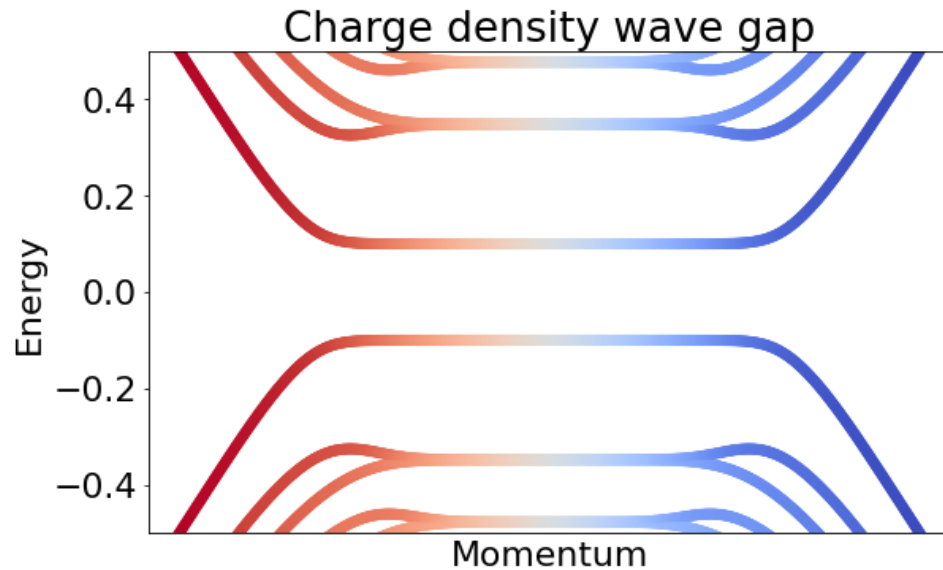
Symmetry breaking the zeroth Landau level gives rise to different topological states

The zeroth Landau level in graphene



The sublattice polarization of the 0th LL allows opening two different gaps in the QH regime

Two topologically trivial gaps in the graphene quantum Hall state

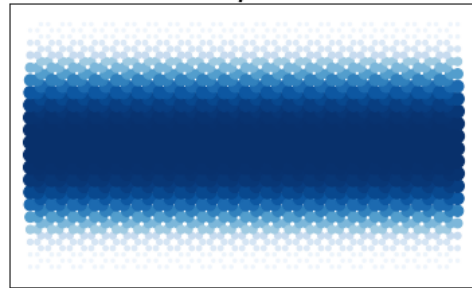


Both CDW and canted antiferromagnetism lead to gapped system without edge modes

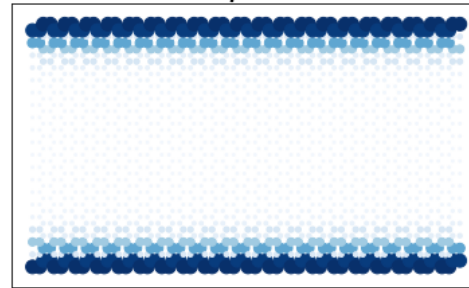
Location of the edge states in the quantum Hall state in graphene

States at zero energy for different chemical potentials in a Chern insulator

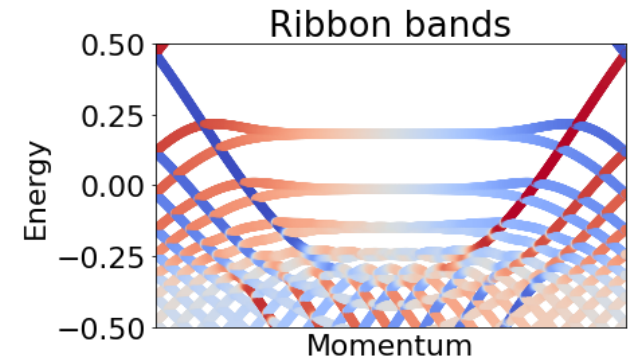
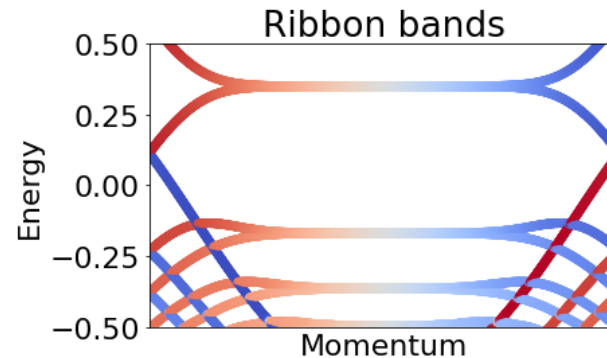
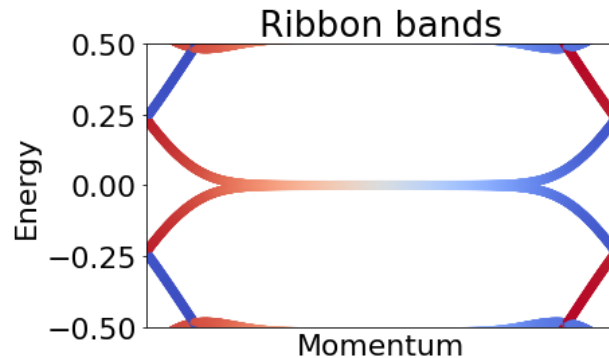
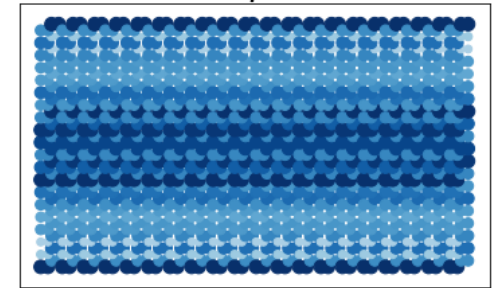
LDOS, $\mu = 0.0$



LDOS, $\mu = 0.35$

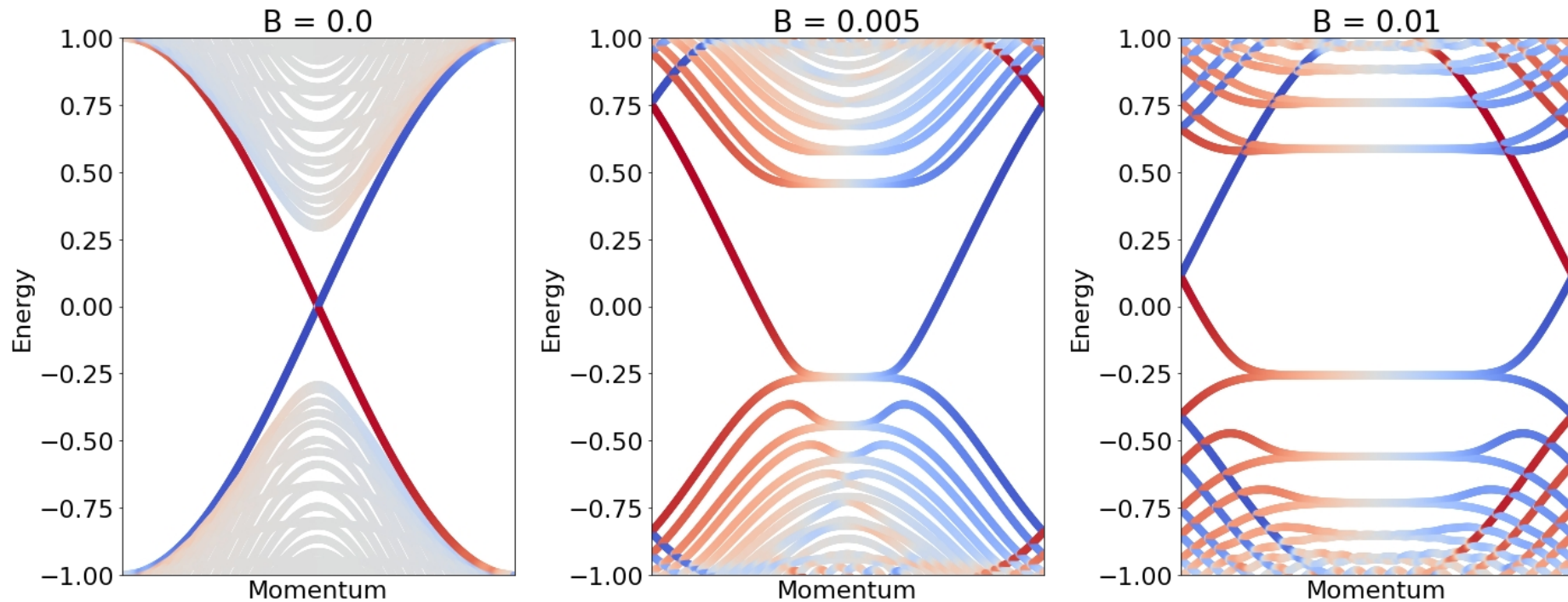


LDOS, $\mu = 0.7$



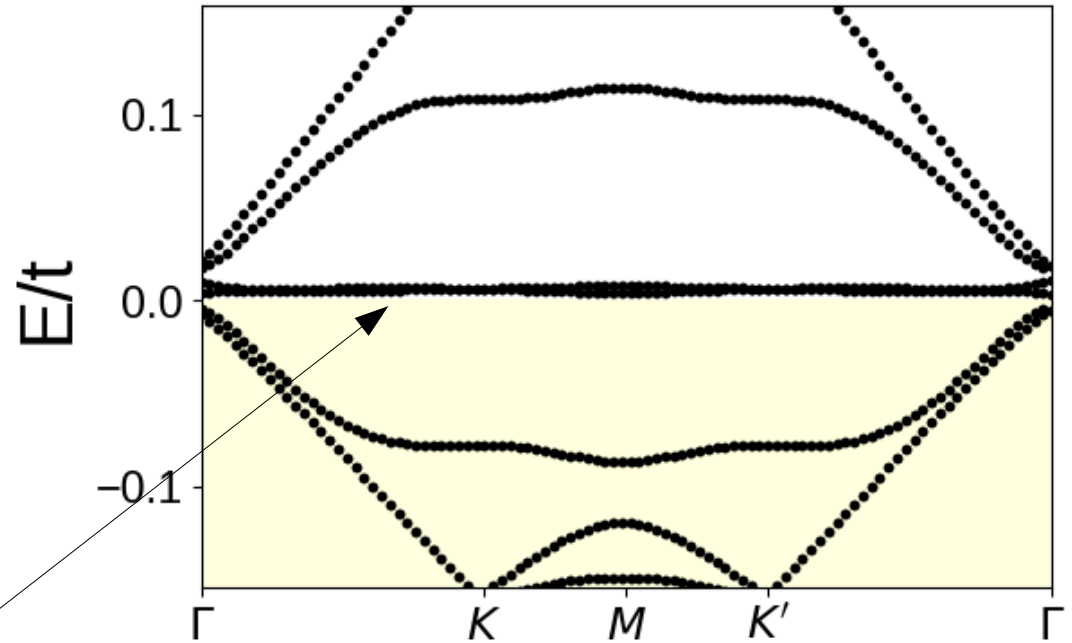
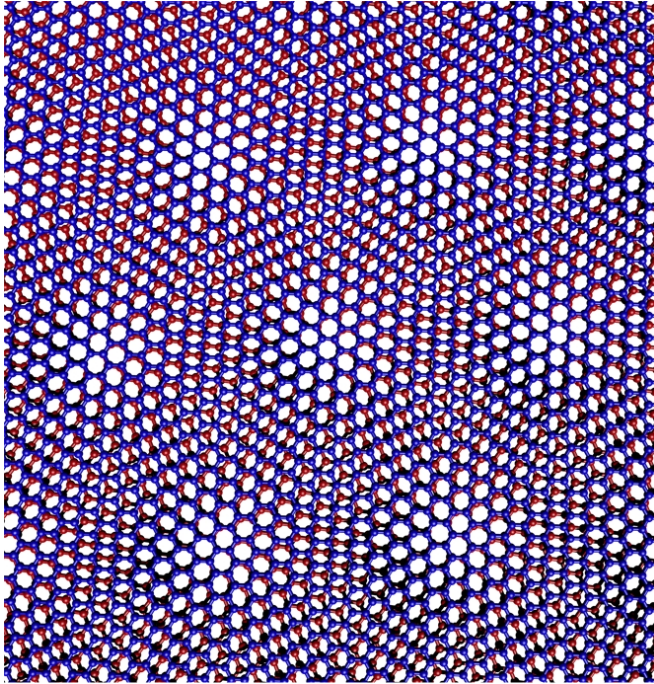
States between LL are located at the edge, while LL are located in the bulk

From a Chern insulator to a quantum Hall state



If one starts if a Chern insulator, the chiral edge states become the quantum Hall edge modes

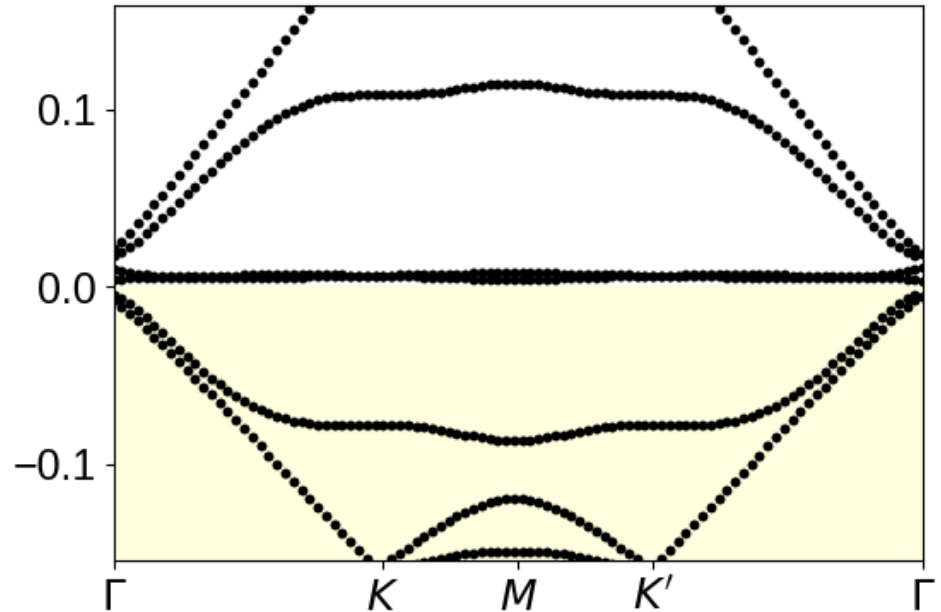
Chern insulators in twisted graphene bilayers



The flat bands of twisted bilayers are pseudo Landau levels

Chern insulators in twisted graphene bilayers

Interactions in twisted bilayers give rise to a valley polarized state, with finite Chern number

 $C = 1$
 $C = 1$
 $C = -1$
 $C = -1$
 $C = 1$
 E/t


hBN encapsulation allows to lift the Dirac points

Van der Waals quantum spin Hall insulators

Edge states in quantum spin Hall insulators

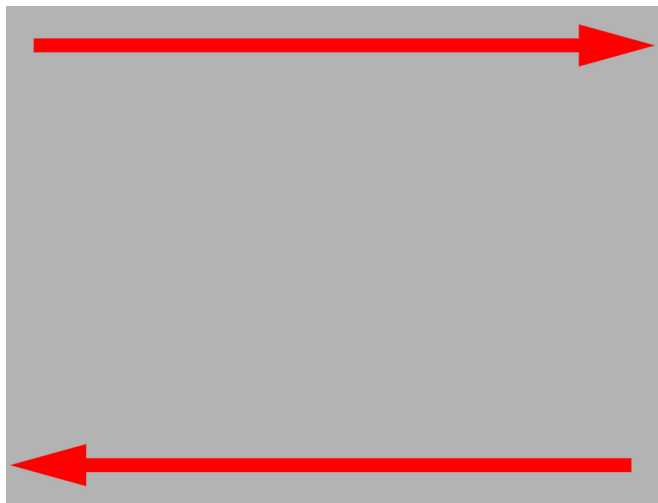
In a quantum spin Hall insulator, opposite spin propagate in opposite directions



Two copies of a quantum Hall insulator, one for each spin channel

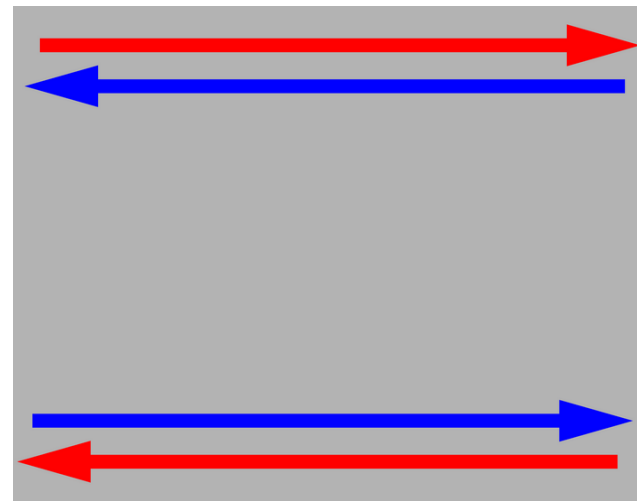
The relation between two topological states

Chern insulators



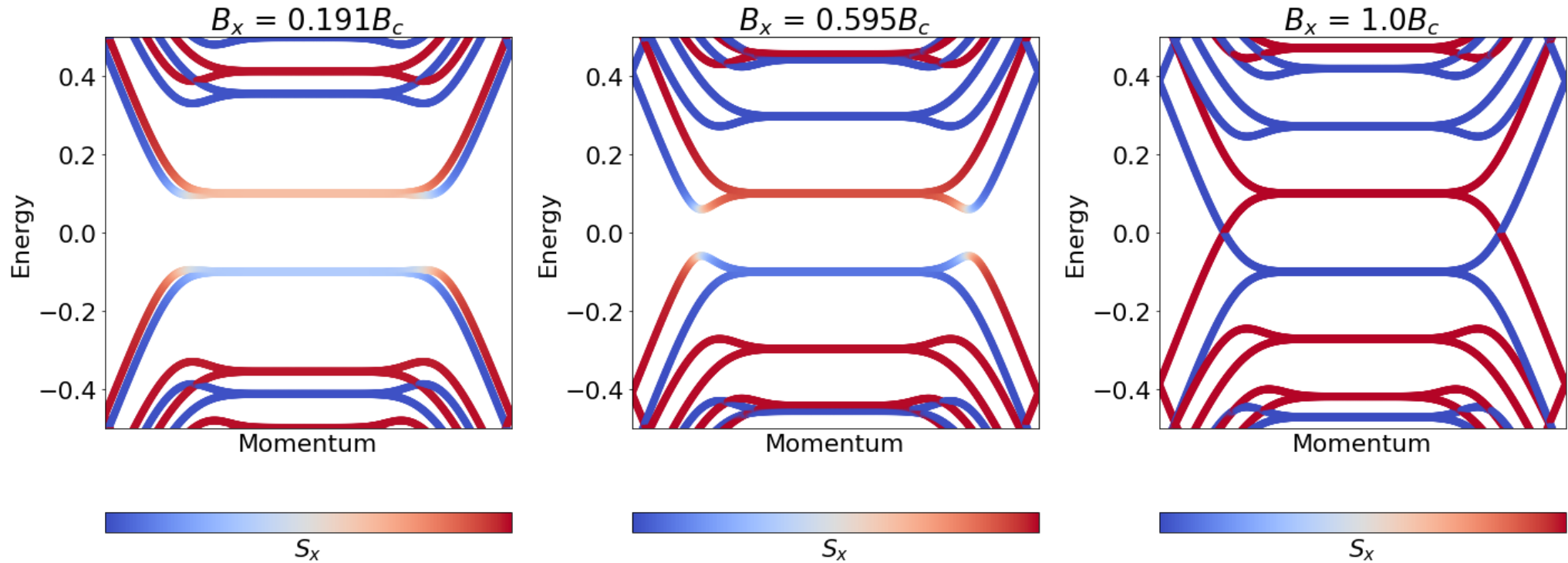
Chiral modes
Break time-reversal symmetry

Quantum spin Hall insulators



Helical modes
Do not break time-reversal symmetry

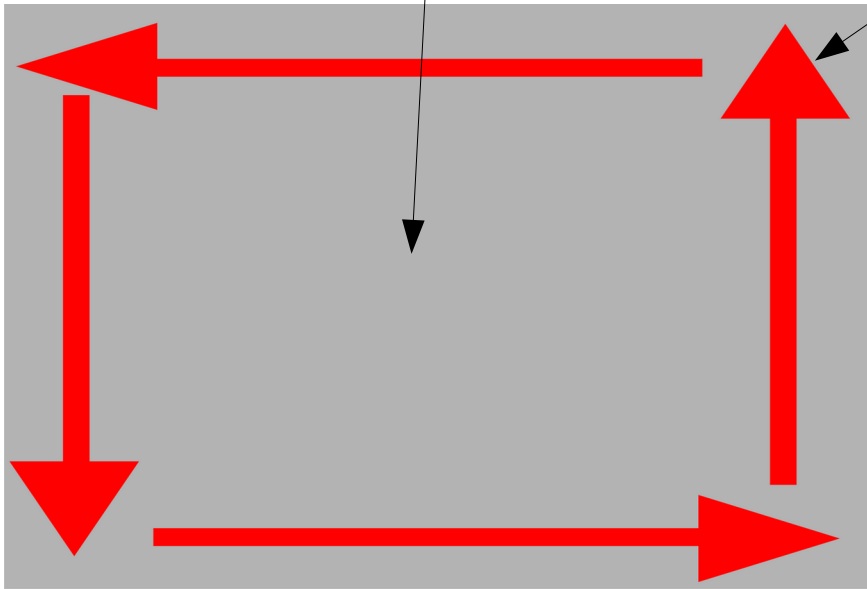
The quantum spin Hall state driven by magnetic field in graphene



As an in-plane field is increased, a trivial QH state transforms into a quantum spin Hall state

Chern insulators

The bulk is insulating



**The edge has chiral states
(without an external magnetic field)**

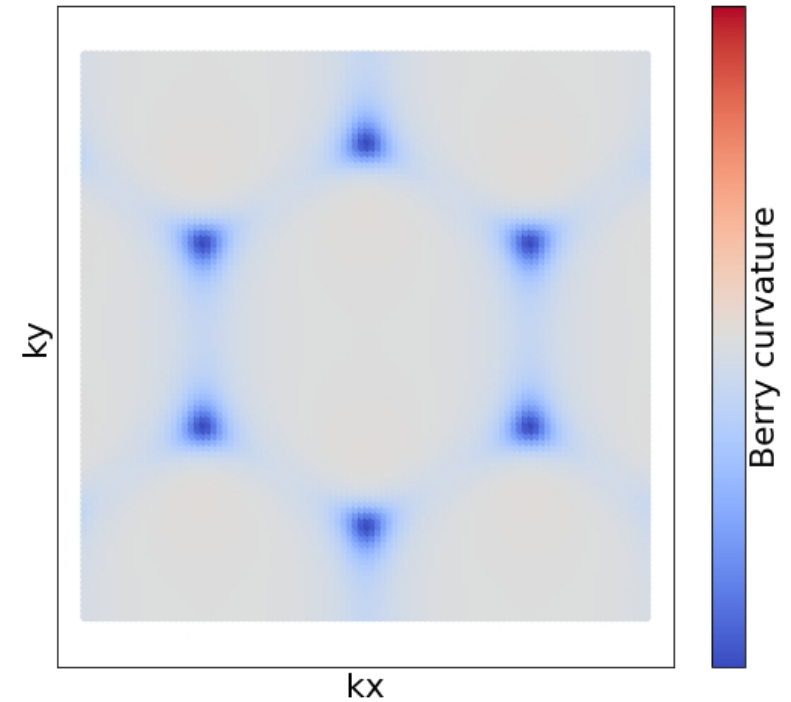
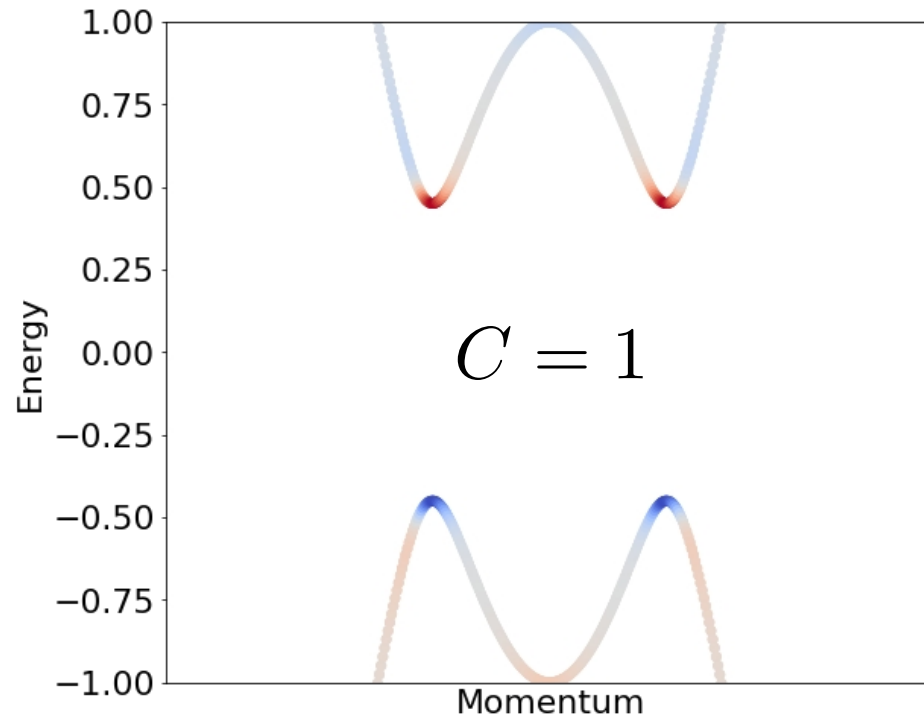
Hall conductivity (Chern number)

$$\sigma_{xy} = \sum_{\alpha \in occ} \int \Omega_{\alpha} d^2 \mathbf{k} = \sum_{\alpha} C_{\alpha} = C$$

$$\Omega_{\alpha} = \partial_{k_x} A_y^{\alpha} - \partial_{k_y} A_x^{\alpha}$$

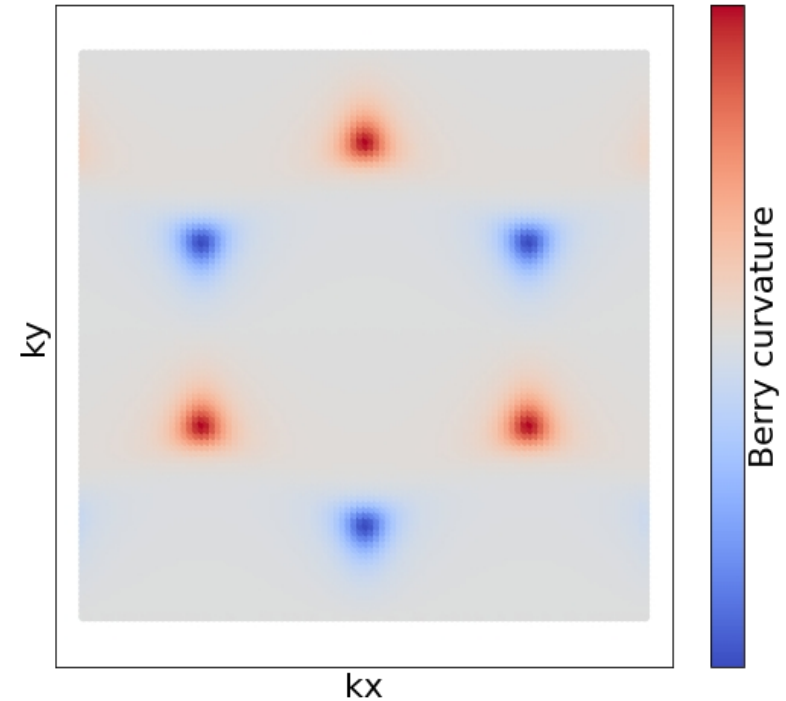
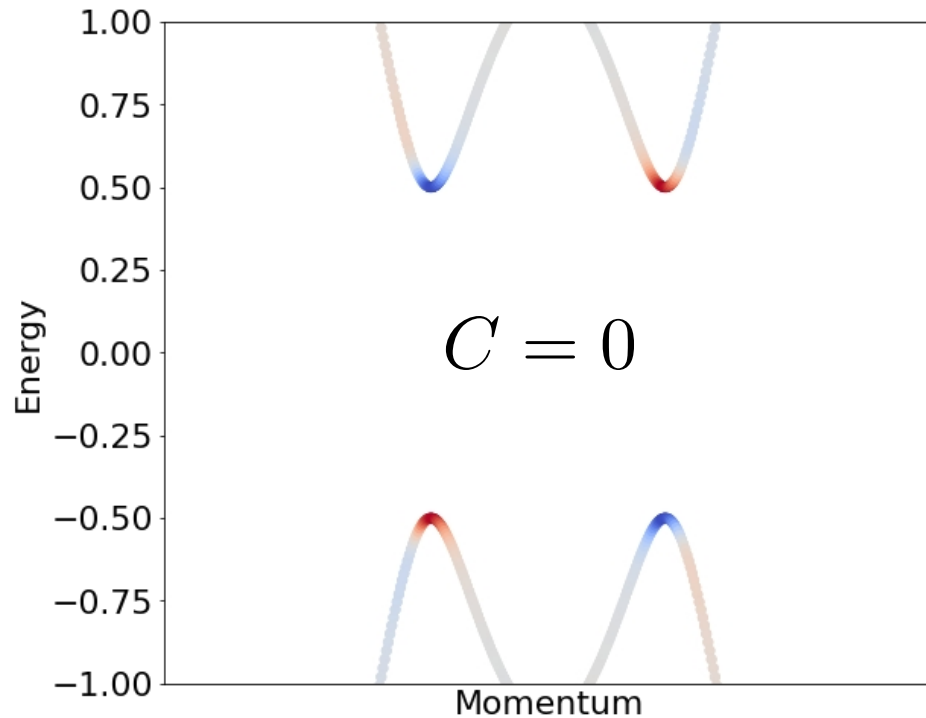
$$A_{\mu}^{\alpha} = i \langle \partial_{k_{\mu}} \Psi_{\alpha} | \Psi_{\alpha} \rangle$$

Two different gaps in a 2D material



The total Chern number is nonzero, driven by breaking of time-reversal symmetry

Two different gaps in a 2D material



The total Chern number is zero, driven by breaking of inversion symmetry

The Hamiltonian of a topological insulator

Look for a system that has massive Dirac equations

$$H(p_x, p_y) = p_x \sigma_x + p_y \kappa \sigma_y + m \sigma_z = \begin{pmatrix} m & p_x + i\kappa p_y \\ p_x - i\kappa p_y & -m \end{pmatrix}$$

The finite mass gives rise to a local Chern number $C_{s,\alpha} = \frac{1}{2} \text{sign}(m) \text{sign}(\kappa)$

If the mass for spin up is opposite than for spin down, then

Chern number

$$C = C_{\uparrow} + C_{\downarrow} = 0$$

Spin Chern number

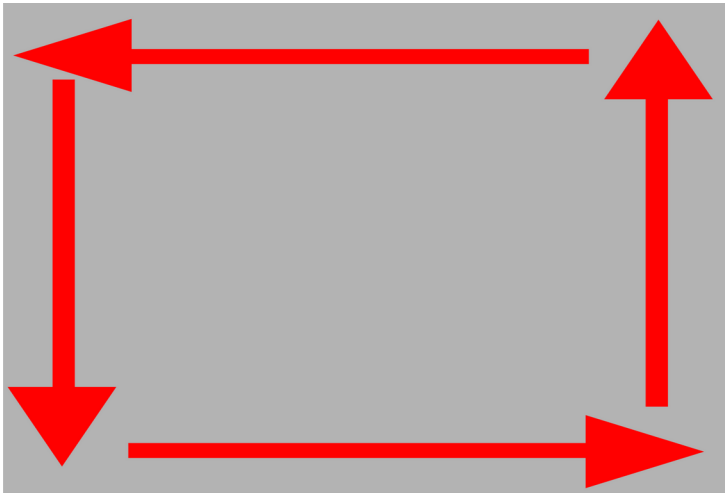
$$C_S = C_{\uparrow} - C_{\downarrow} = \pm 2$$

In a system with spin-orbit coupling, spin dependent masses can be generated

Quantum spin Hall insulators

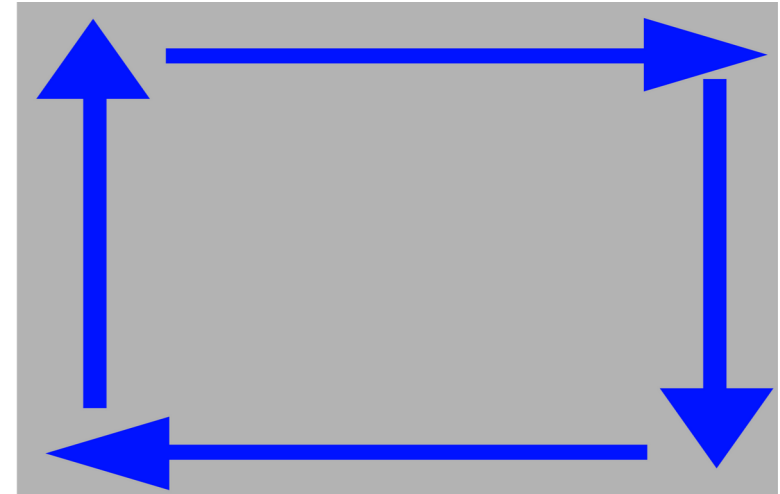
Chern insulator for spin up

$$C^{\uparrow} = 1$$



Chern insulator for spin down

$$C^{\downarrow} = -1$$



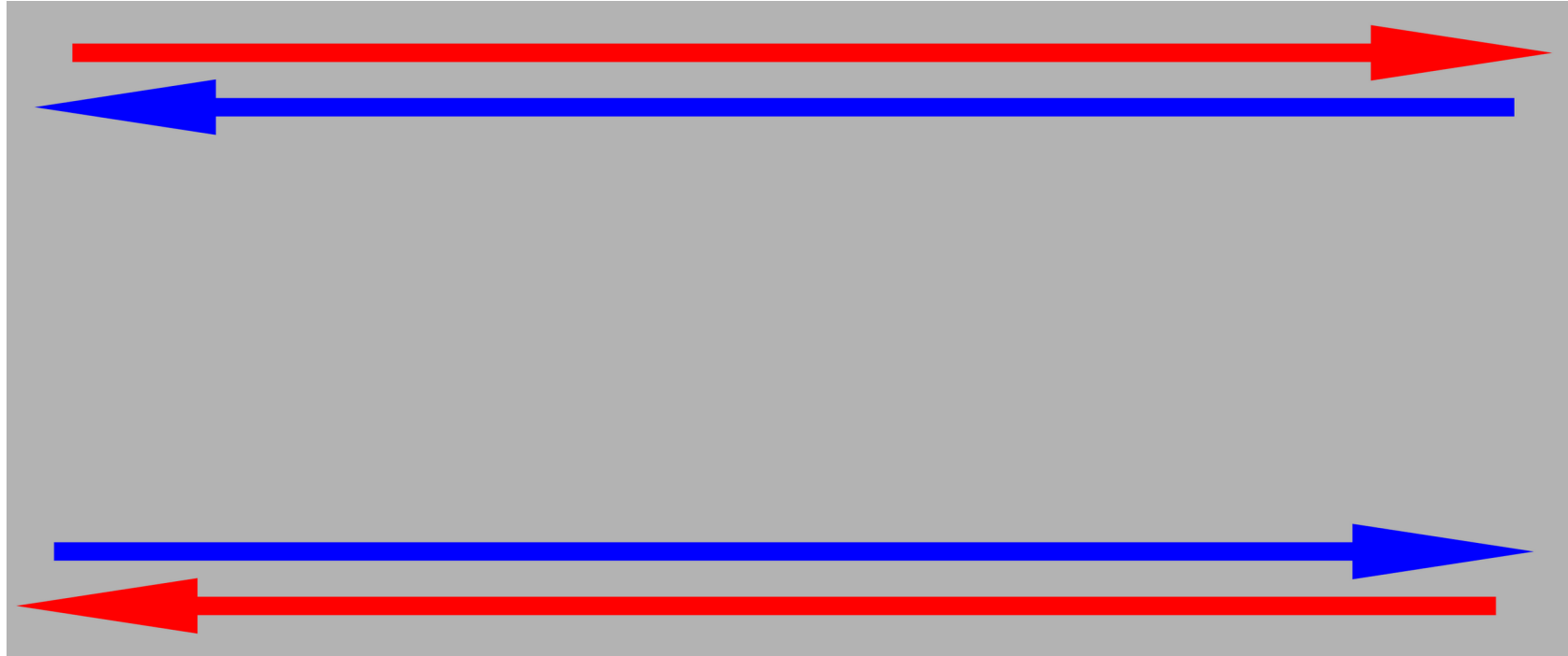
Spin-orbit coupling (SOC) can drive a quantum spin Hall state

$$\vec{L} \cdot \vec{S} \sim L_z S_z \quad \text{SOC acts as a magnetic field with opposite signs for opposite spins}$$



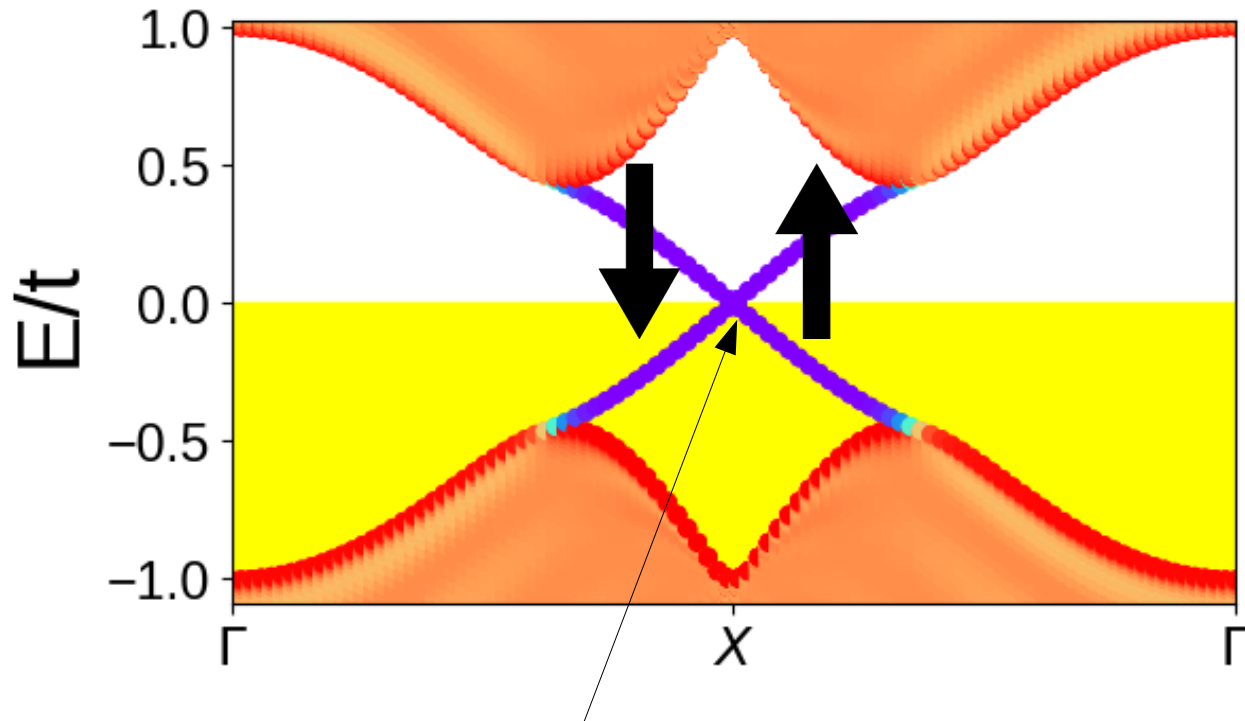
Quantum spin Hall insulators

Opposite spins propagate in opposite directions (helical gas)





Quantum spin Hall insulators



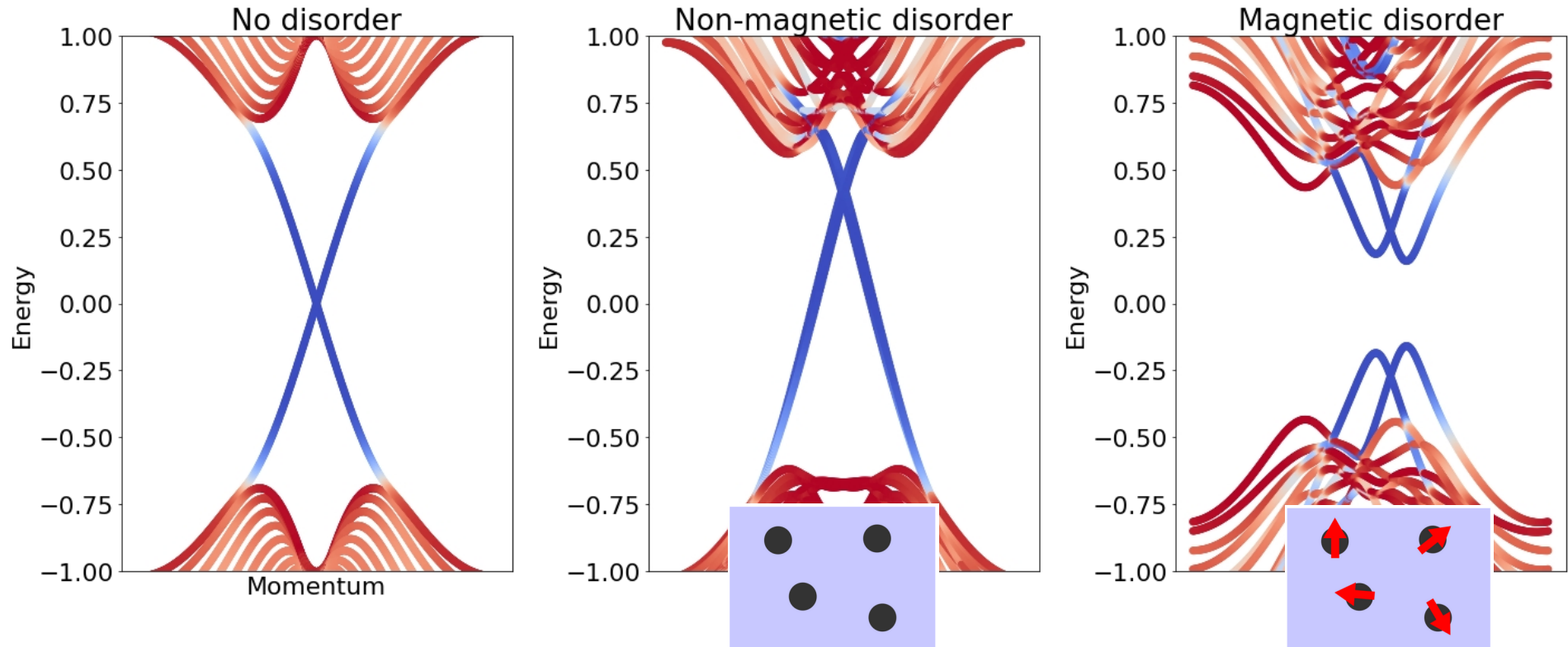
The gapless nature is protected by Kramer's theorem

$1T\text{-WTe}_2$

Time-reversal
symmetry

$$\Theta^2 = -1$$

Disorder in quantum spin Hall insulators



Disorder that breaks time reversal symmetry opens a gap in the topological states

Break

10-15 min break

(optional) to discuss during the break

Which of the two schematics depicts a correct interface between a Chern and spin Hall insulator?

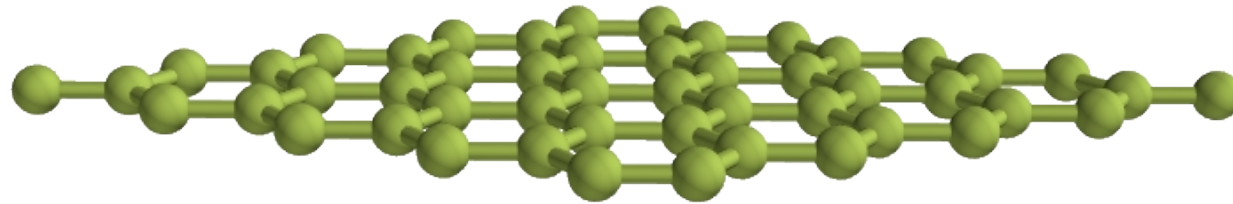


Valley Chern insulators 2D materials

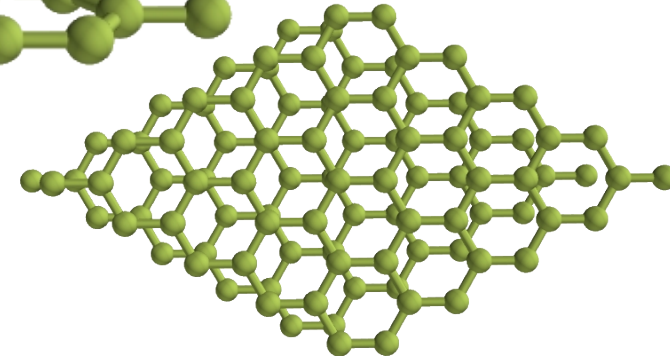
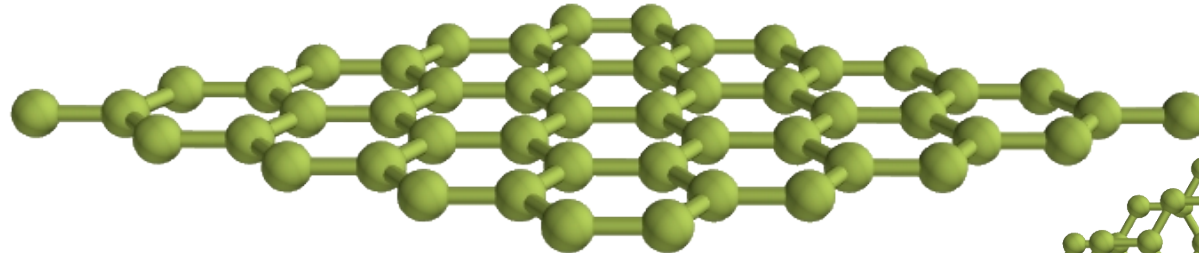
The structure of bilayer graphene

Let us now focus on a graphene bilayer with AB stacking

$$+Ec_n^\dagger c_n$$



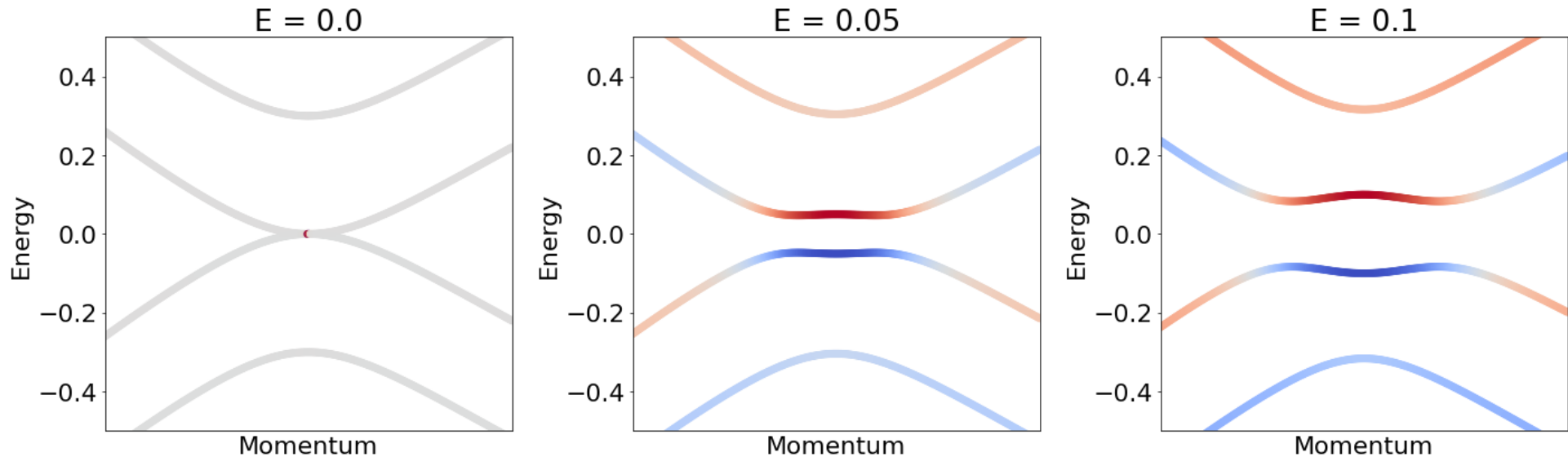
$$-Ec_n^\dagger c_n$$



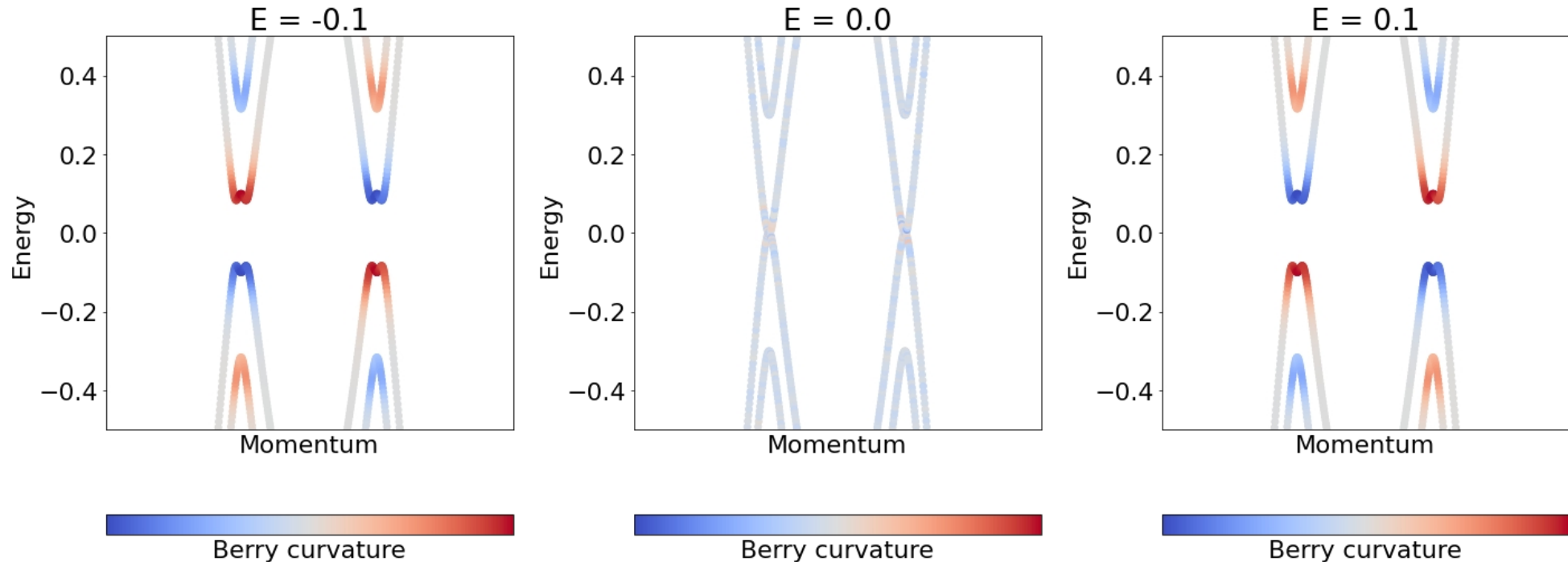
And we will add an interlayer bias

The electronic structure of bilayer graphene

Graphene bilayers open a gap when an interlayer bias is applied



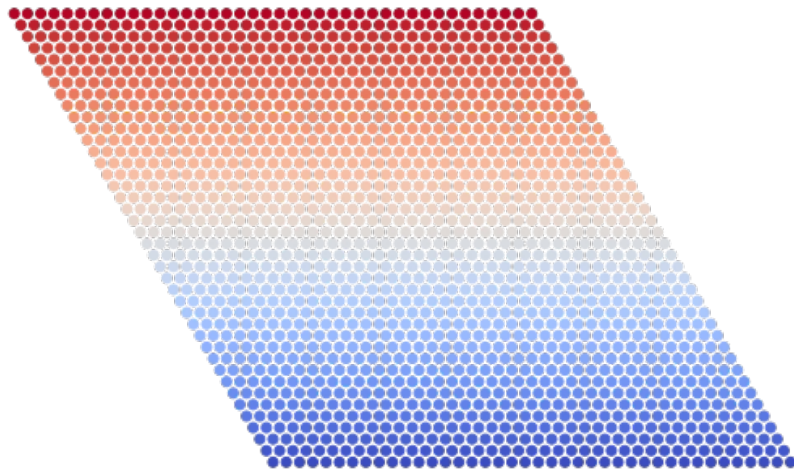
Electrically controllable topology in graphene bilayers



The Berry curvature of the bands is controllable with an interlayer bias

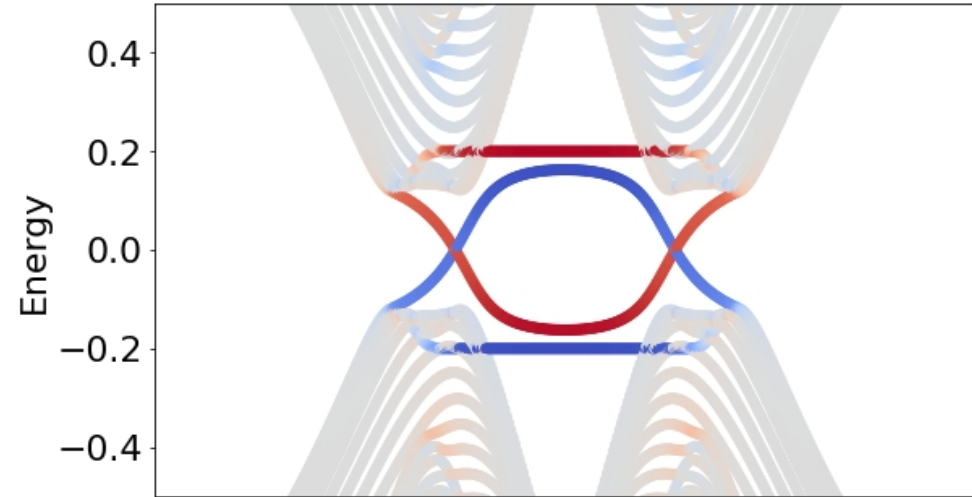
Biased bilayer graphene, pseudo-helical states

Position operator



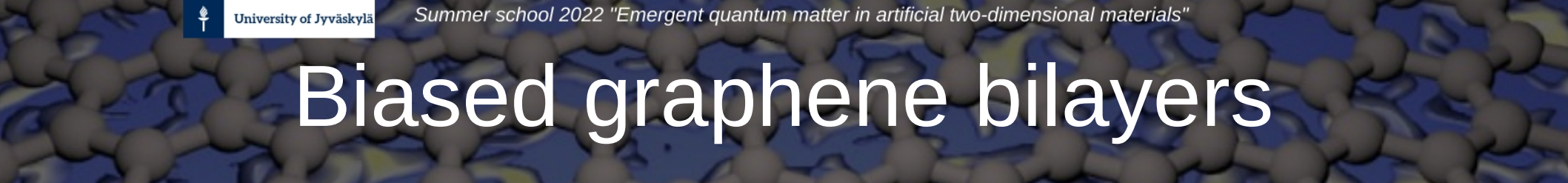
edge/bulk/edge

Band structure



edge/bulk/edge

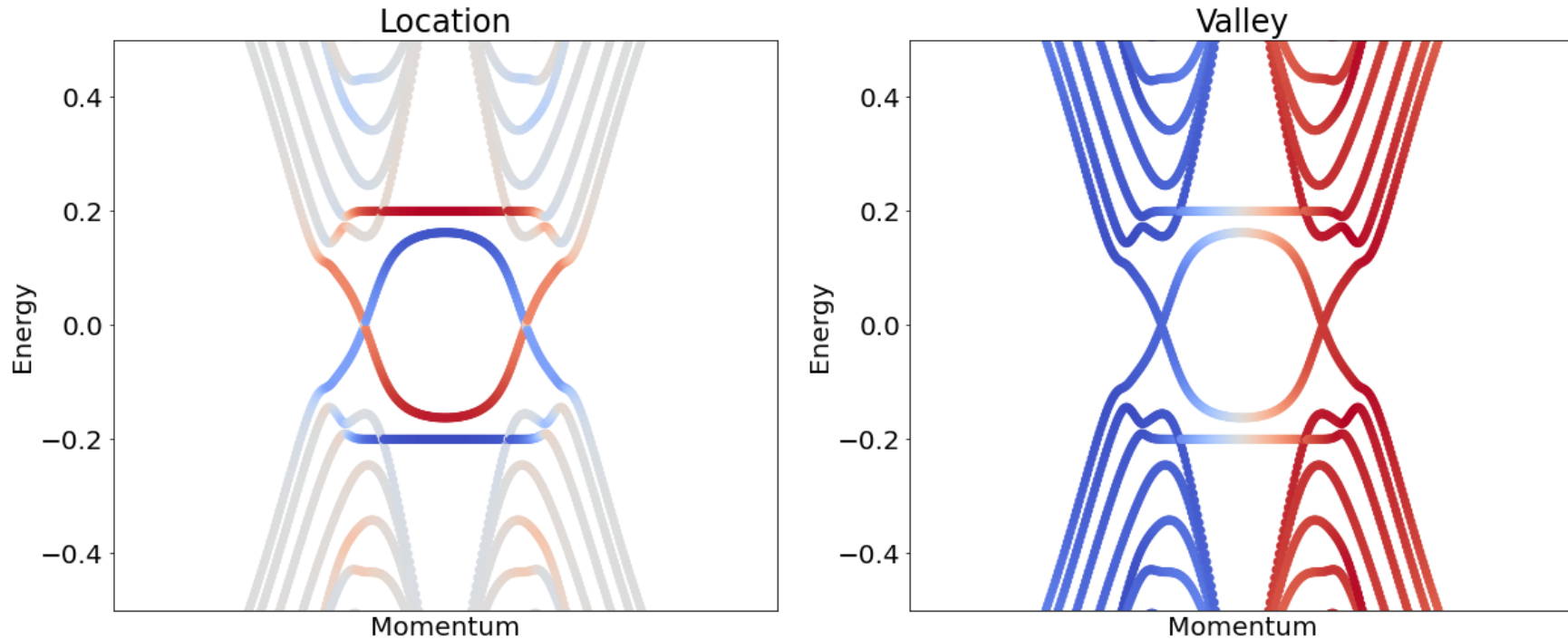
Edge states appear in the presence of a bias between layers



University of Jyväskylä

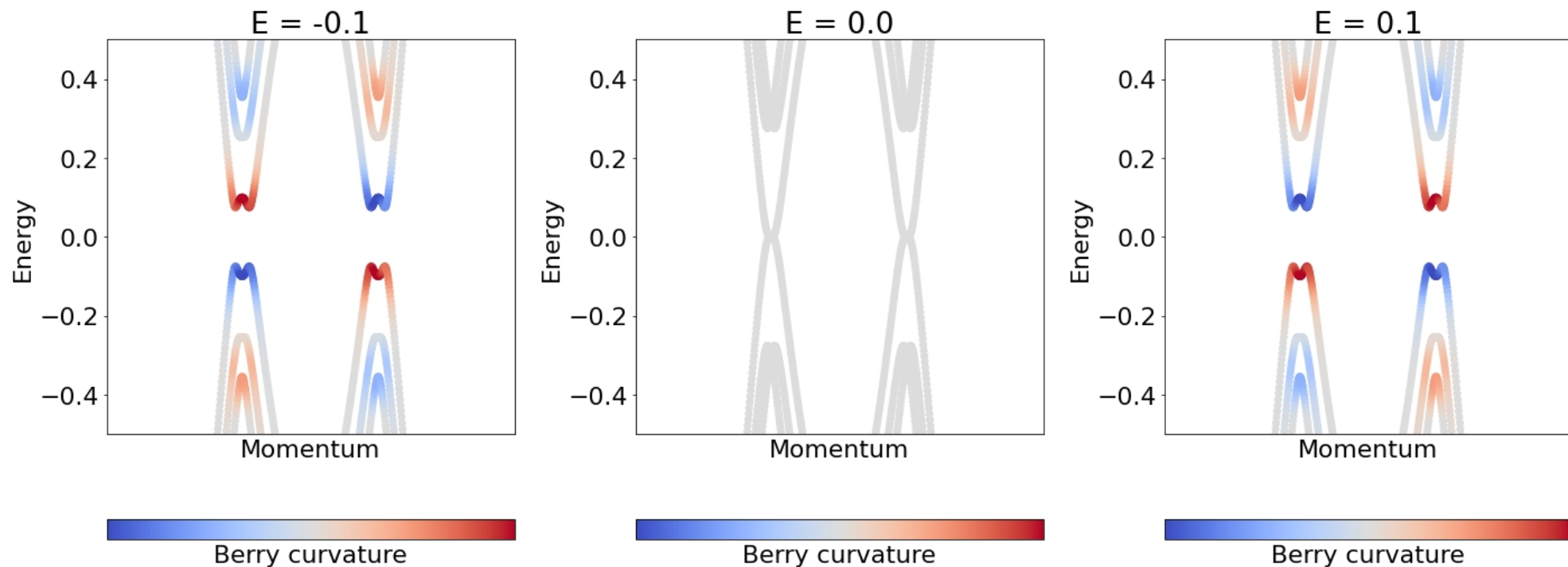
Summer school 2022 "Emergent quantum matter in artificial two-dimensional materials"

Biased graphene bilayers



A valley Hall state generates counter propagating pseudo-helical modes

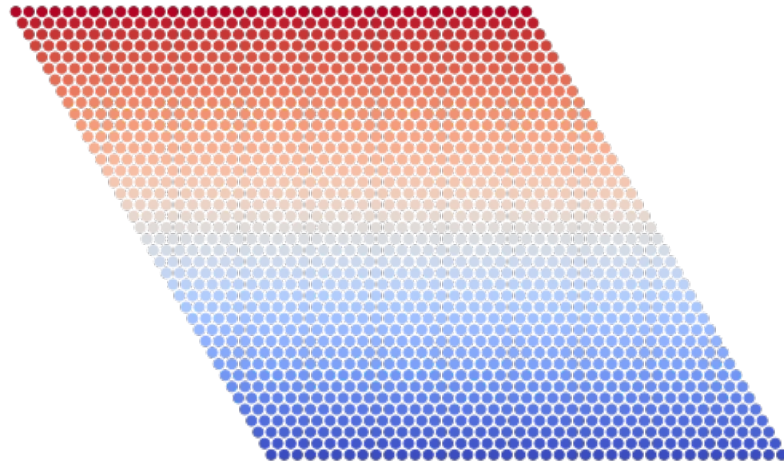
Bias controlled electronic structure in ABC trilayer graphene



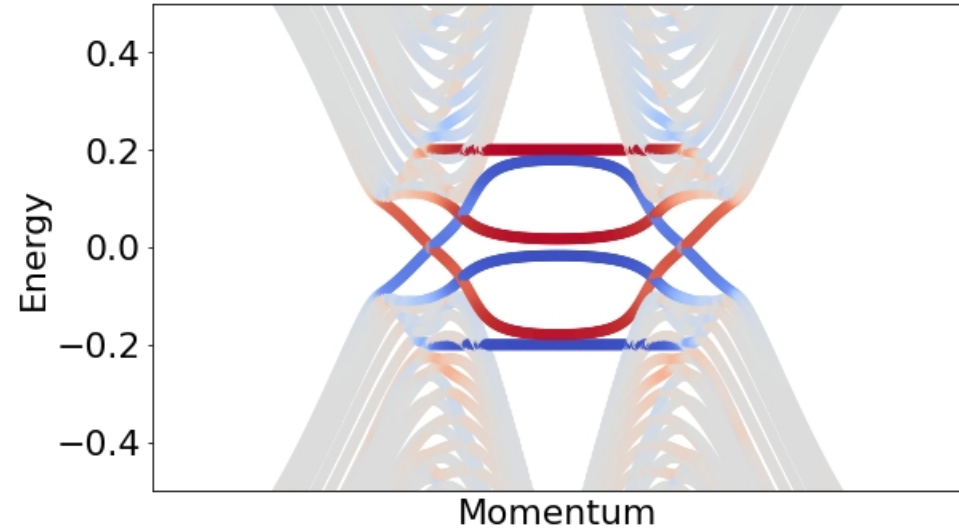
The Berry curvature of the bands is controllable with an interlayer bias

Valley Hall states in ABC graphene multilayers

Position operator



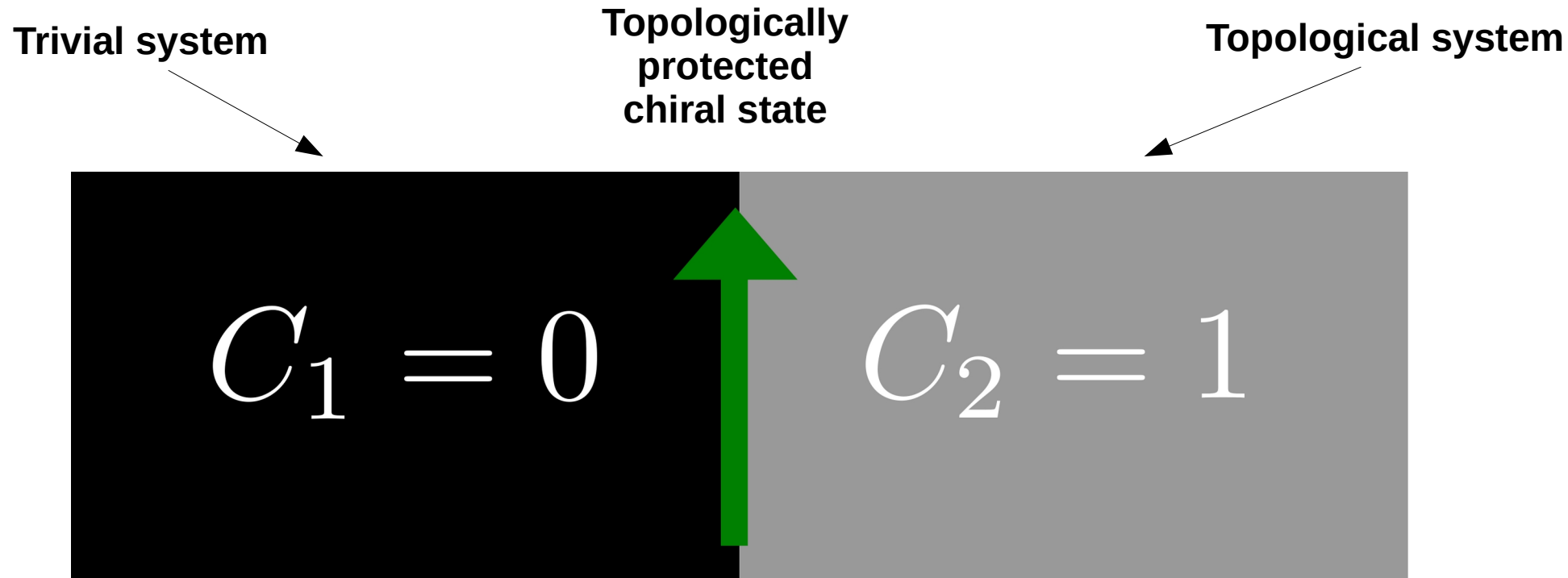
Band structure



Other graphene multilayers sub ABC trilayer also show valley Hall effect with an applied field

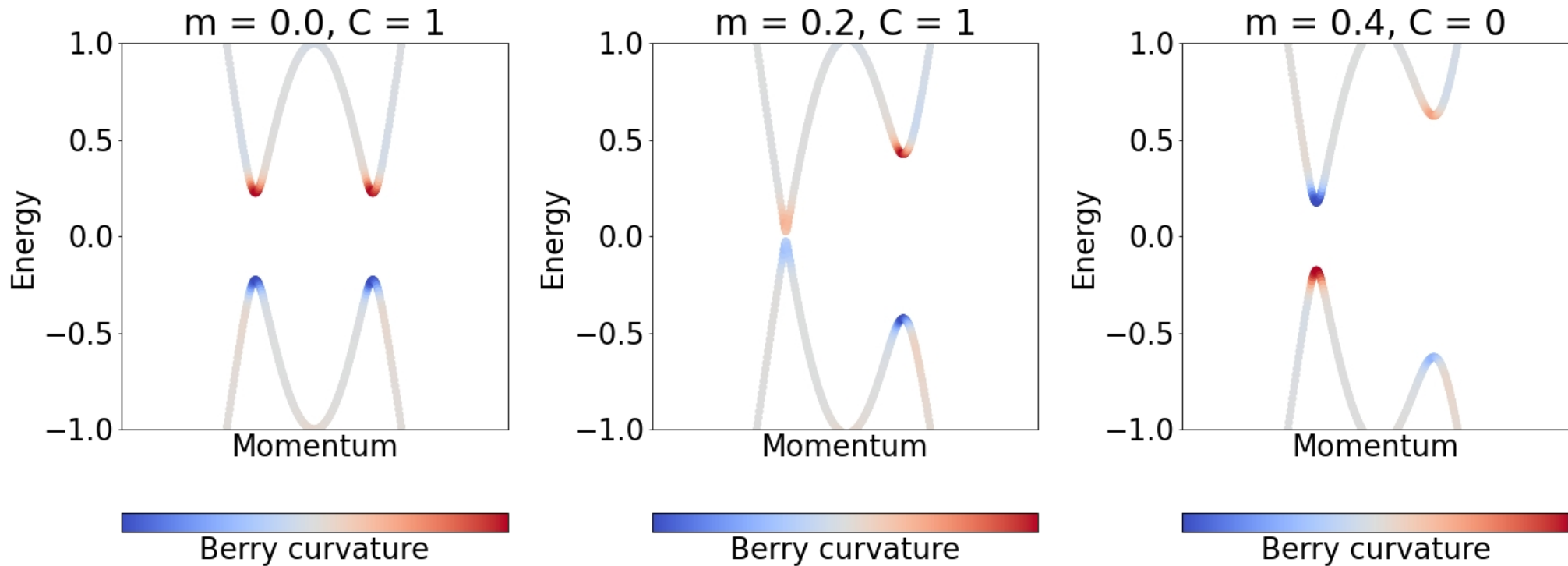
Topological phase transitions

Topological protection and edge states



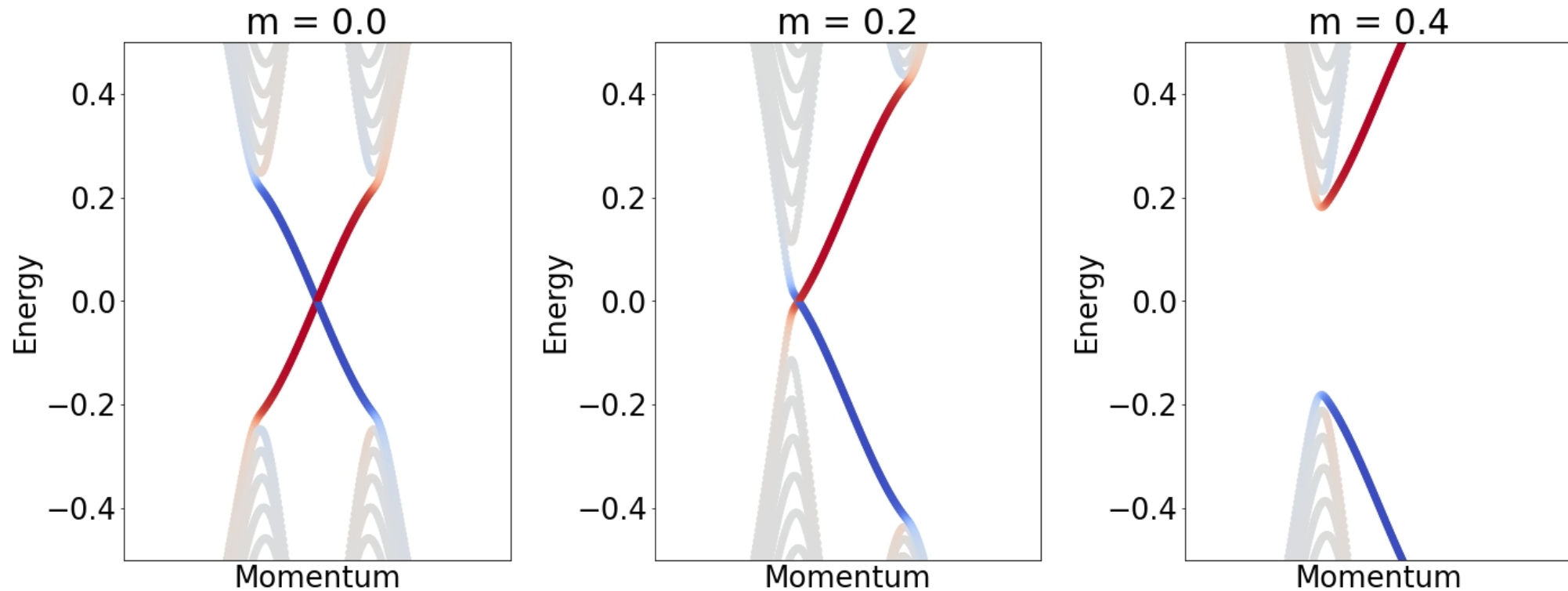
Transforming between Hamiltonians with different topological invariant closes a gap

Topological phase transition in the bulk, Chern insulator



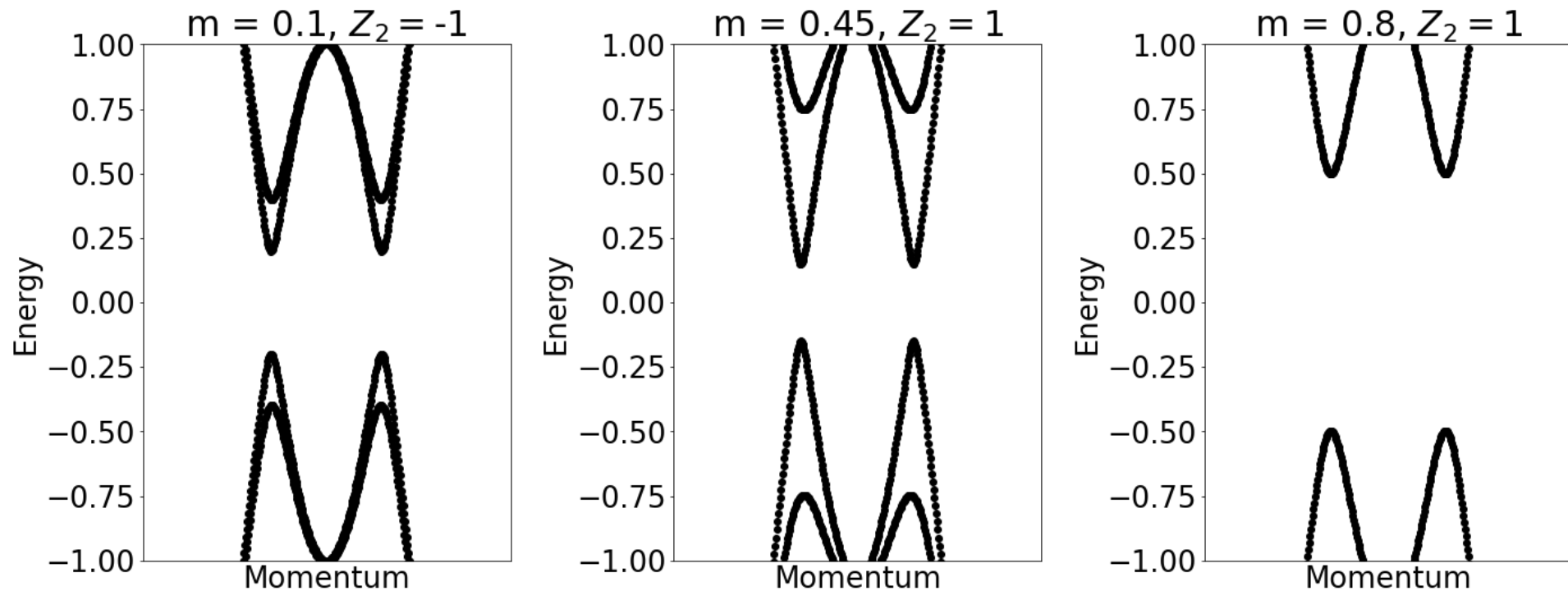
A gap closing in the bulk leads to a change in the Berry curvature of the occupied states

Topological phase transition in the edge, Chern insulator



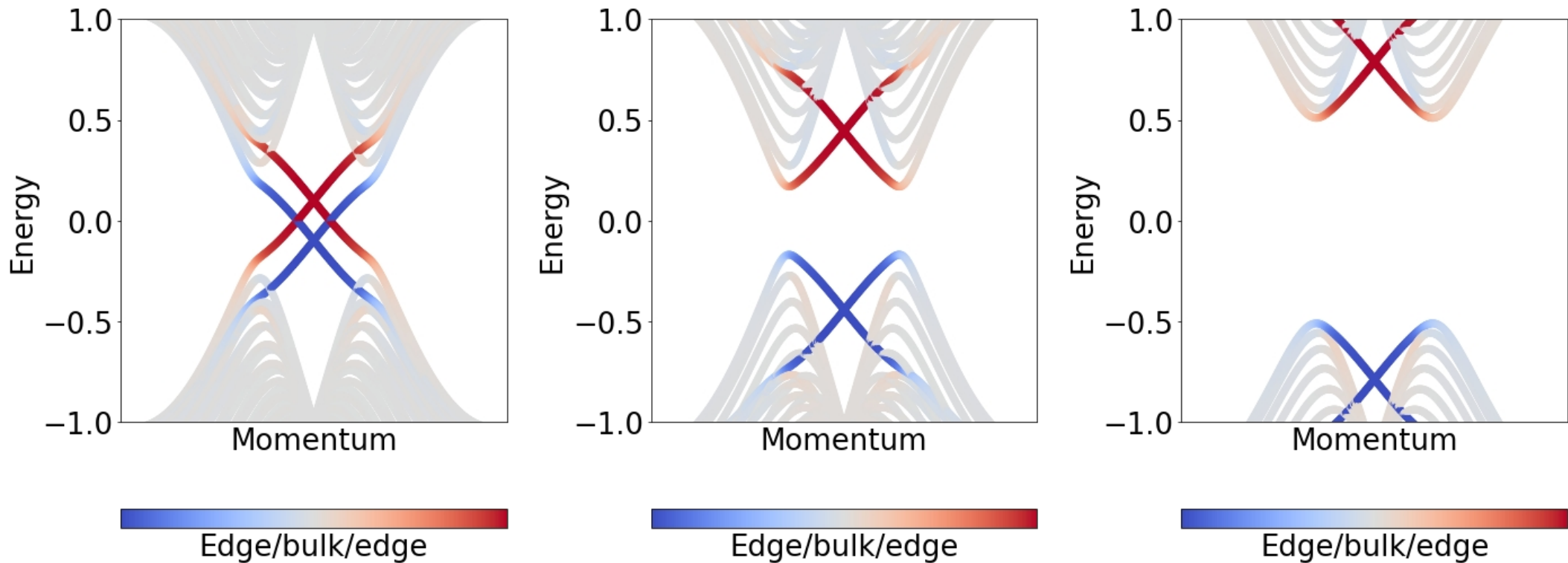
A gap closing in the bulk leads to a change in the chiral edge states

Topological phase transition in the bulk, quantum spin Hall insulator



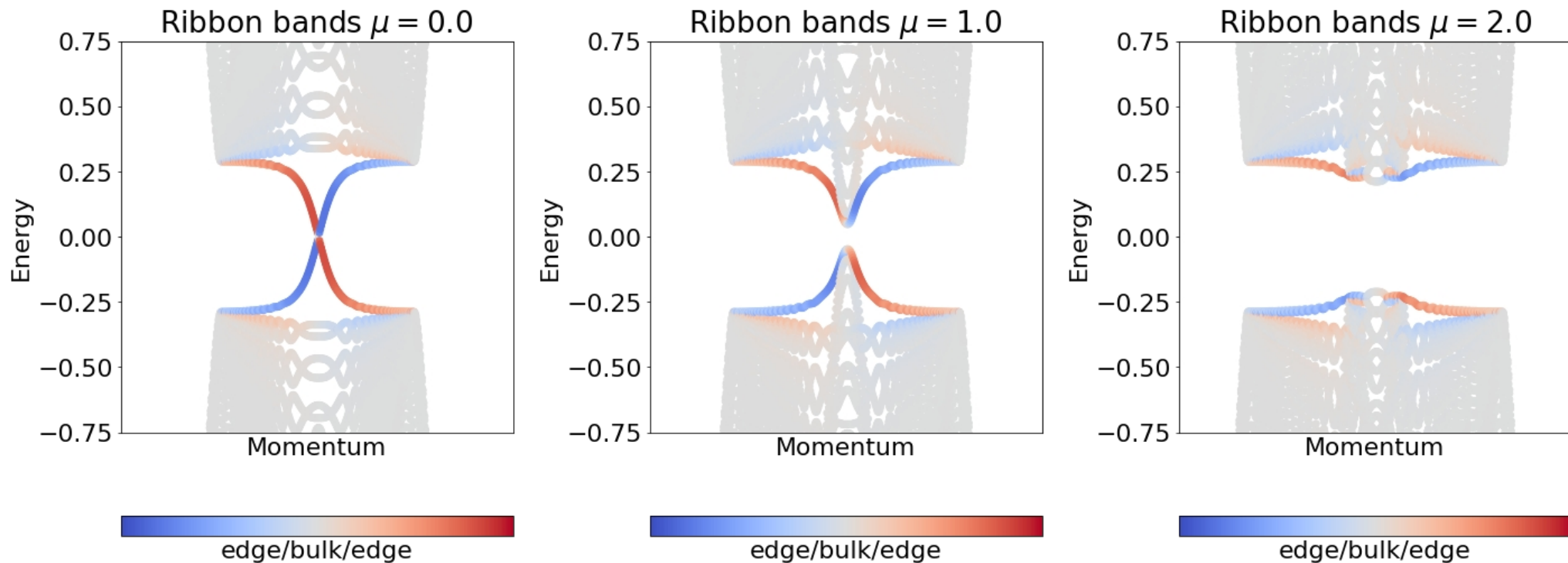
A gap closing in the bulk leads to a change in the Z_2 invariant

Topological phase transition in the edge, quantum spin Hall insulator



A gap closing in the bulk leads to a change in the chiral edge states

Topological phase transition in artificial topological superconductors



As the chemical potential is changed, a transition from topological to trivial takes place

For the exercise session this afternoon

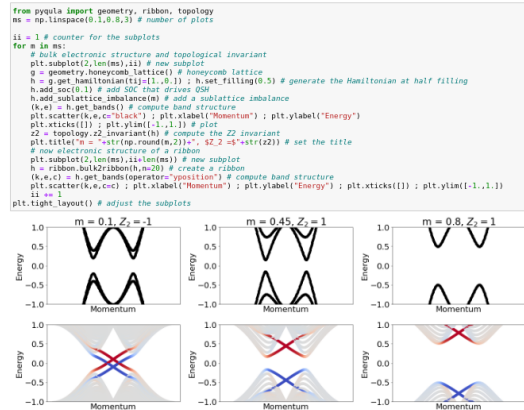
Download the Jupyter-notebook from

https://github.com/joselado/jyvaskyla_summer_school_2022/blob/main/sessions/session5.ipynb

The tasks during the exercise sessions

You will see examples with the code

You have to modify them, and answer questions



Exercise

- Count how many helical states you have in each edge for the 1D system for each case
- Add Rashba spin-orbit coupling (add_rashba). Do you still see the edge states? Discuss why
- Add a second neighbor hopping (g.get_hamiltonian(tij=[1,0,2])). Do you still see the edge states? Discuss why