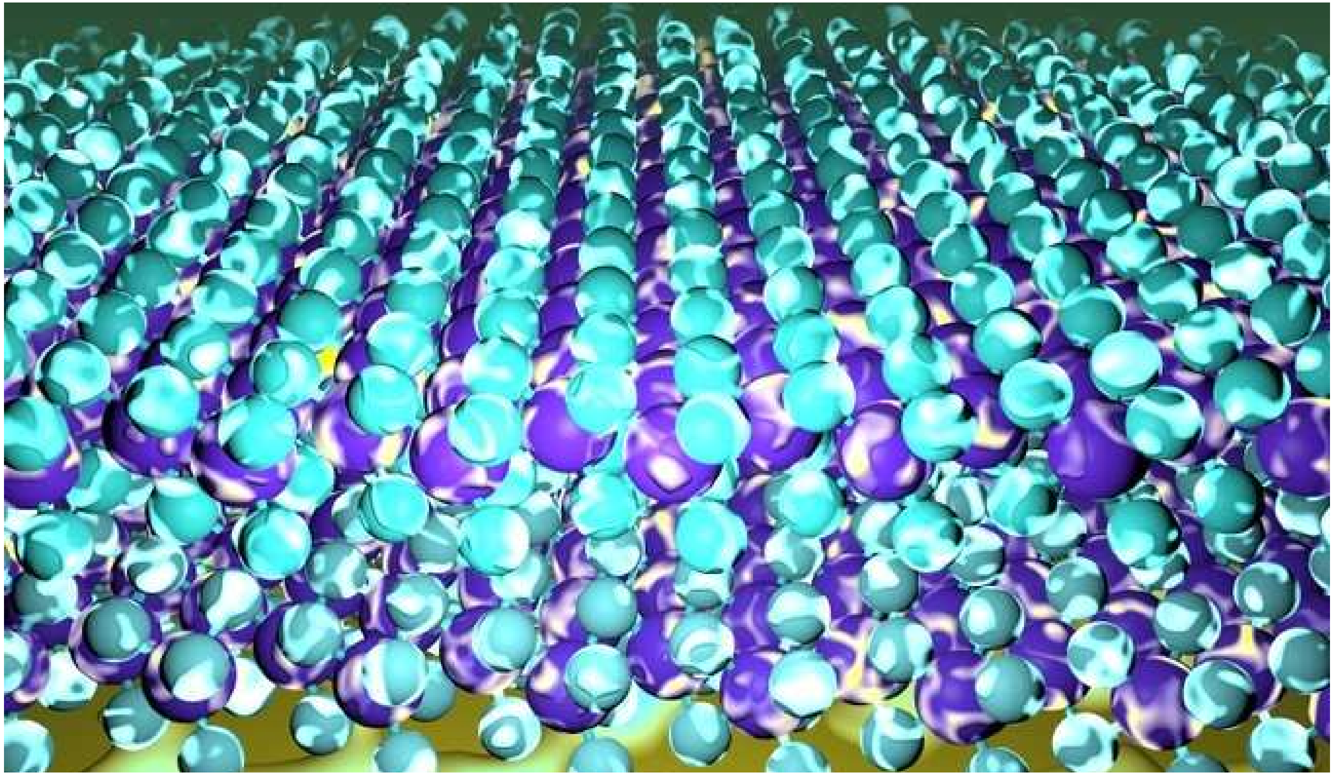
Topological states in van der Waals materials



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

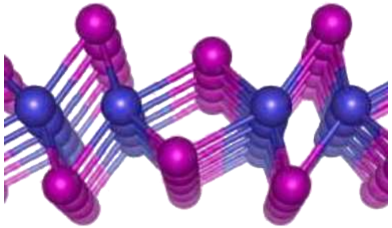
Topological van der Waals materials

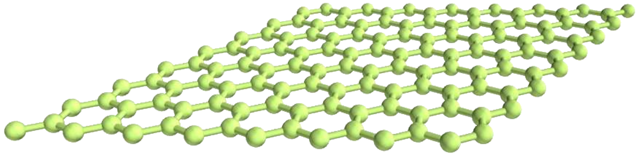
Quantum spin Hall insulators

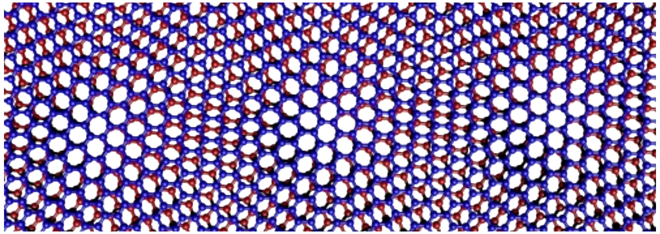
Chern insulators

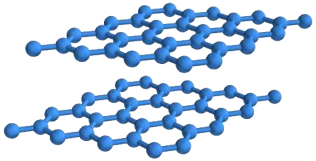
Valley Chern insulators

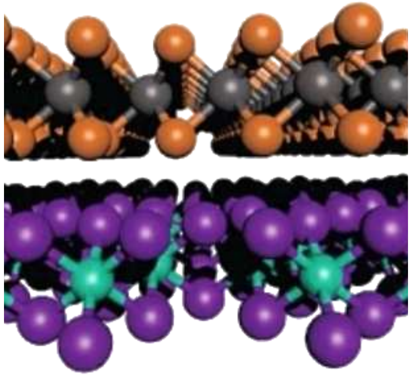
Topological superconductors











1T'-WTe_2

QH graphene

Twisted graphene multilayers

Bilayer graphene

$CrBr_3/NbSe_2$

Preserve time-reversal symmetry/S_z

Break time-reversal symmetry

Preserve valley symmetry

Break gauge symmetry

Topology in electronic systems

Topological invariant in a Hamiltonian

We can classify Hamiltonians according to topological invariants

$$\begin{tikzcd}[column sep=huge, row sep=huge]
\underset{\textbf{Hamiltonian}}{H(\mathbf{k})} \arrow[r] & \underset{\textbf{Wavefunction}}{|\Psi(\mathbf{k})\rangle} \arrow[d] \\
C = \int_{BZ} \Omega d^2\mathbf{k} & \Omega = \nabla \times \mathbf{A}\big|_z \arrow[l]
\end{tikzcd}$$

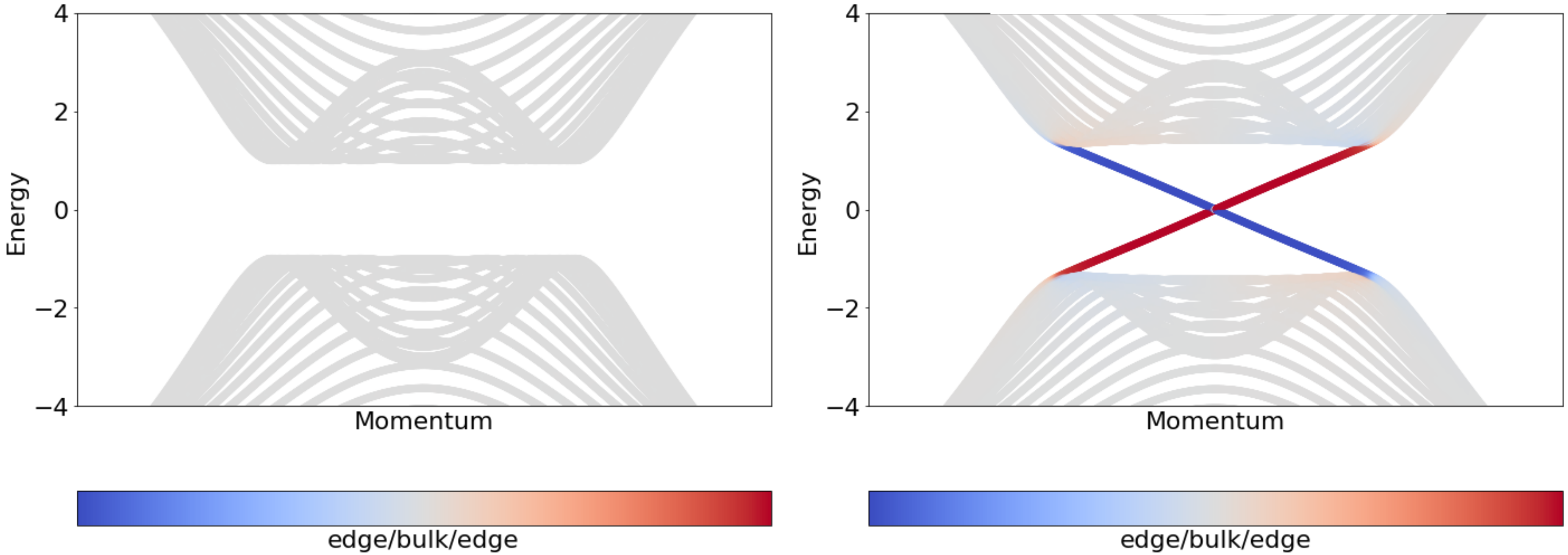
Topological invariant (Chern number)

Metric (Berry curvature)

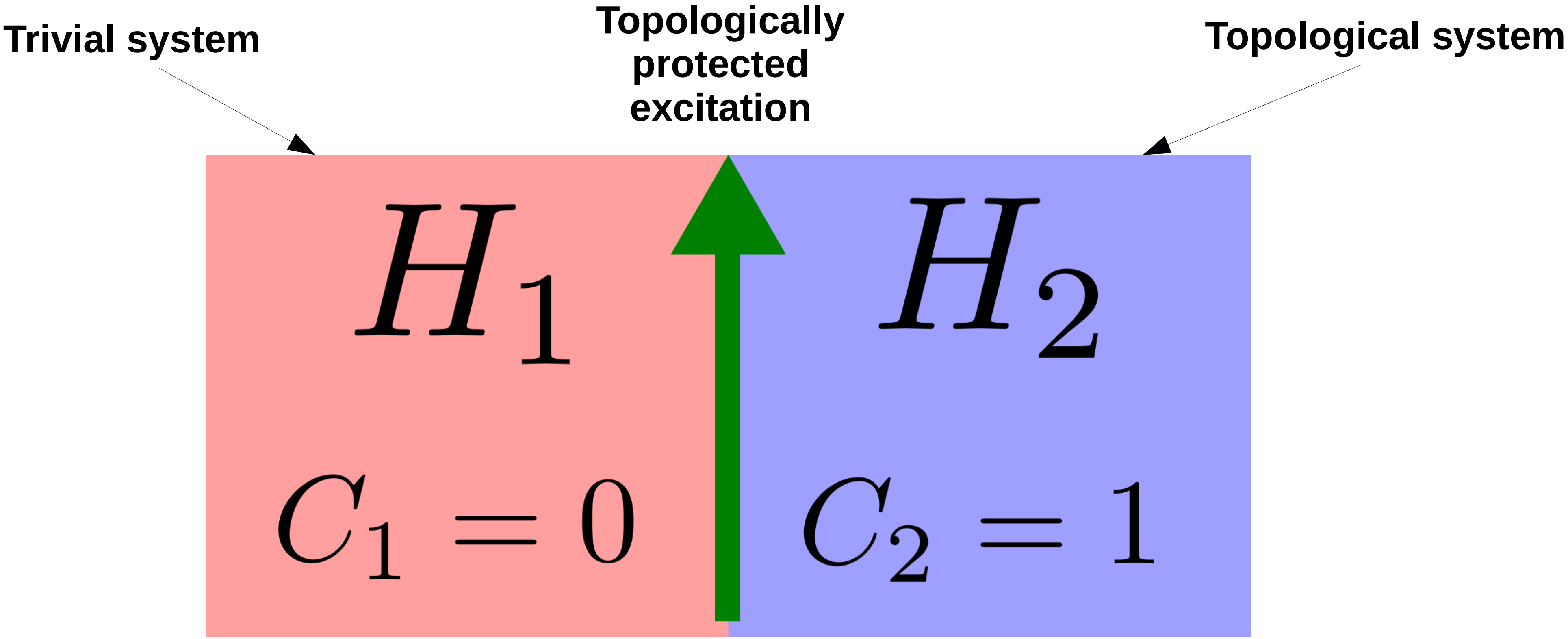
The role of a topological invariant

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

$$C = 0 \qquad\qquad C = 1$$



The consequence of different topological invariants



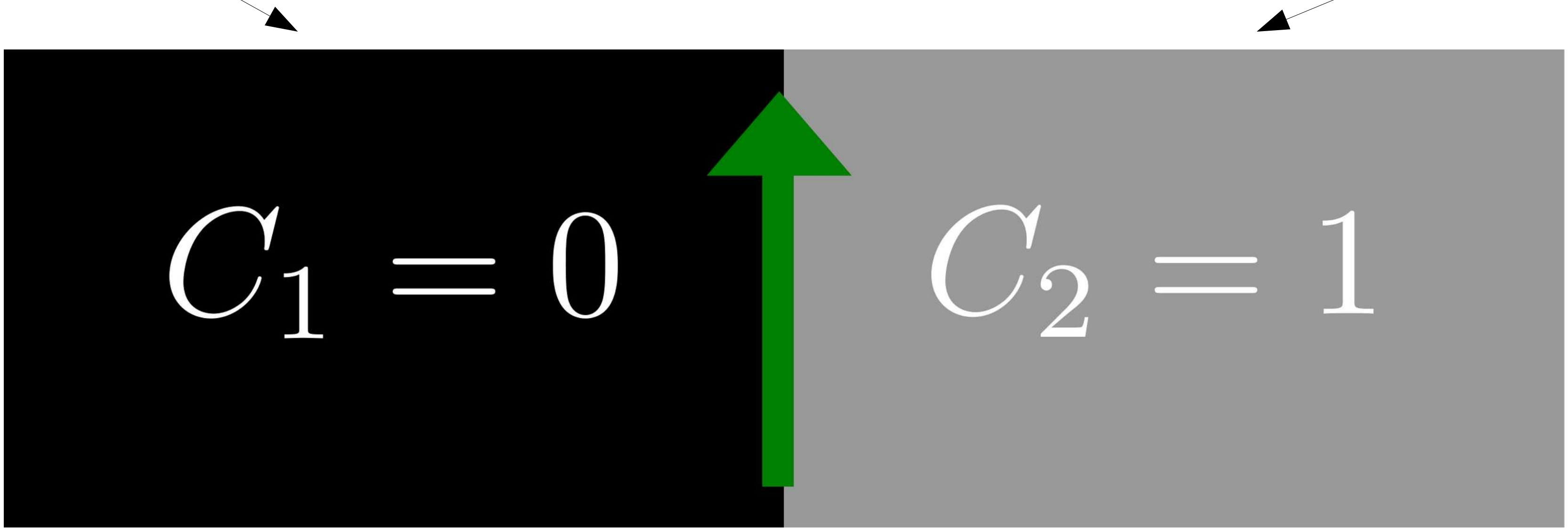
Topological excitations appear between topologically different systems

The edge states of the quantum Hall effect

Trivial system

Topologically protected chiral state

Topological system



The edge states of the quantum Hall effect are topological excitations

The edge states of the quantum Hall effect

No backscattering channel

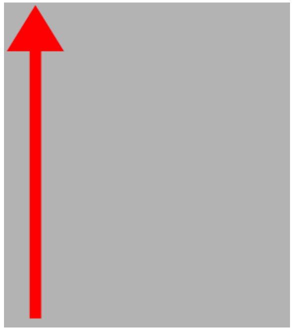
<u>Perfect conductance</u>

Topological protection

<u>The edge states of the quantum Hall effect are topologically protected</u>

Four topological states in 2D materials

Chern insulators

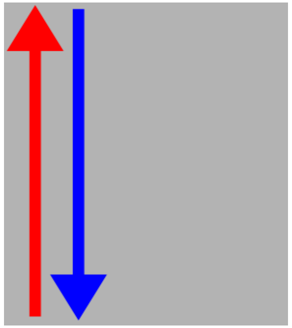


Chiral states

Electronics

Twisted graphene bilayer

Quantum spin Hall insulators

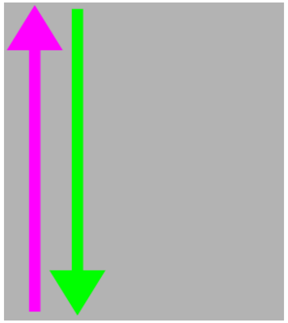


Helical states

Spintronics

1T'-WSe_2

Quantum valley Hall insulators

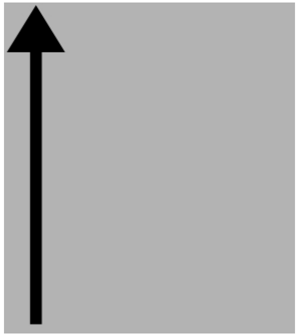


Valley-helical states

Valleytronics

Bilayer graphene

Topological superconductors



Majorana excitations

Topological quantum computing

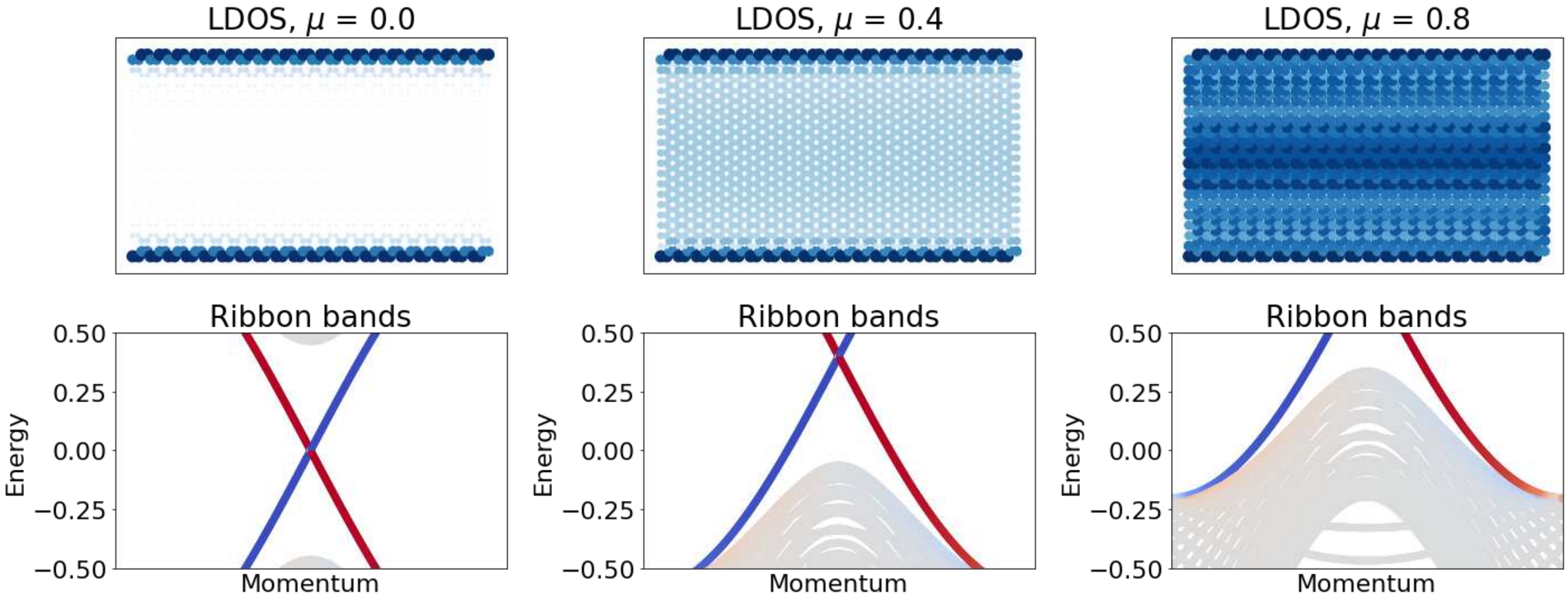
$CrBr_3/NbSe_2$

Four topological states in 2D materials

Chern insulators	**Quantum spin Hall insulators**	**Quantum valley Hall insulators**	**Topological superconductors**
$C = 0, 1, 2, ...$	$Z_2 = 0, 1$	$C_V = 0, 1, 2, ...$	$C = 0, 1, 2, ...$
Chern number	Z_2 invariant	Valley Chern number	Chern number
Twisted graphene bilayer	1T'-WSe_2	Bilayer graphene	*$CrBr_3/NbSe_2$*

Location of states in a Chern insulator

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



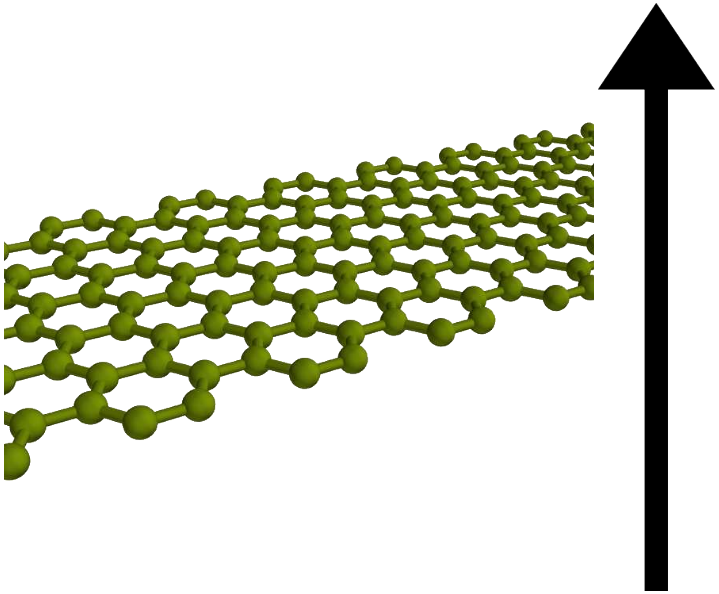
States in the gap are located at the edge, where above the gap states are located in the bulk

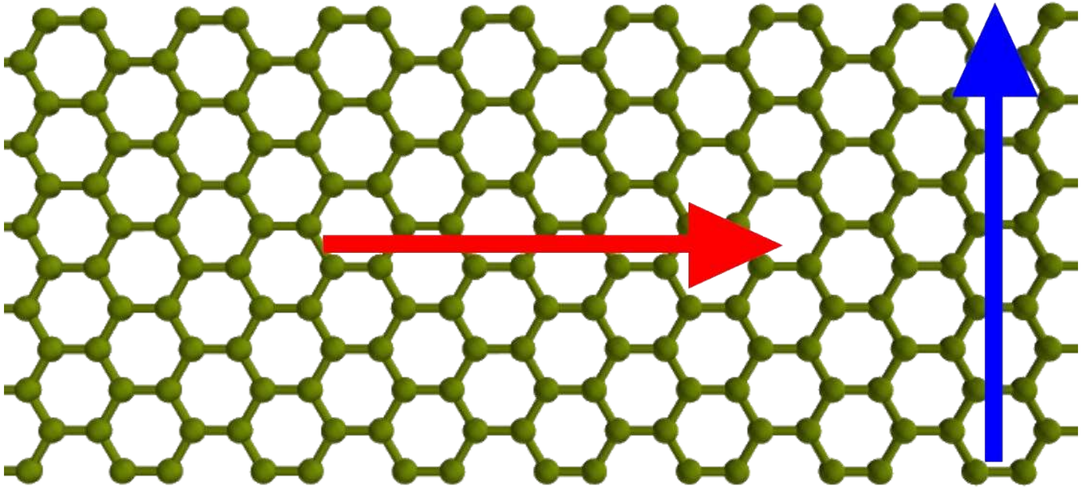
The quantum Hall effect

The quantum Hall effect

Take graphene in the presence of a very large magnetic field

Measure a current in x





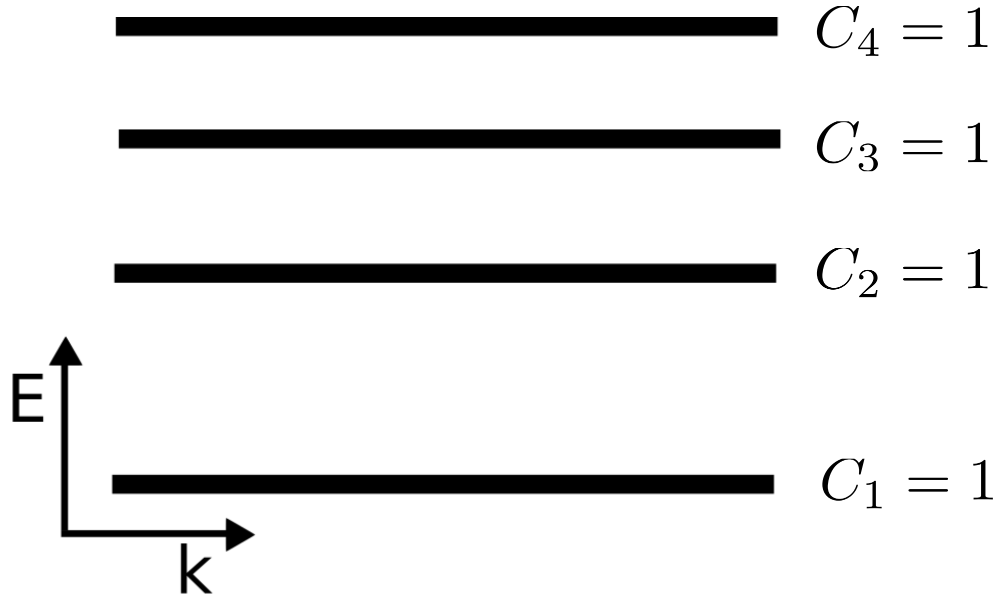
Apply a voltage in y

Apply a magnetic field in z

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

The quantum Hall effect

Band-structure in the quantum Hall state



Hall conductivity

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

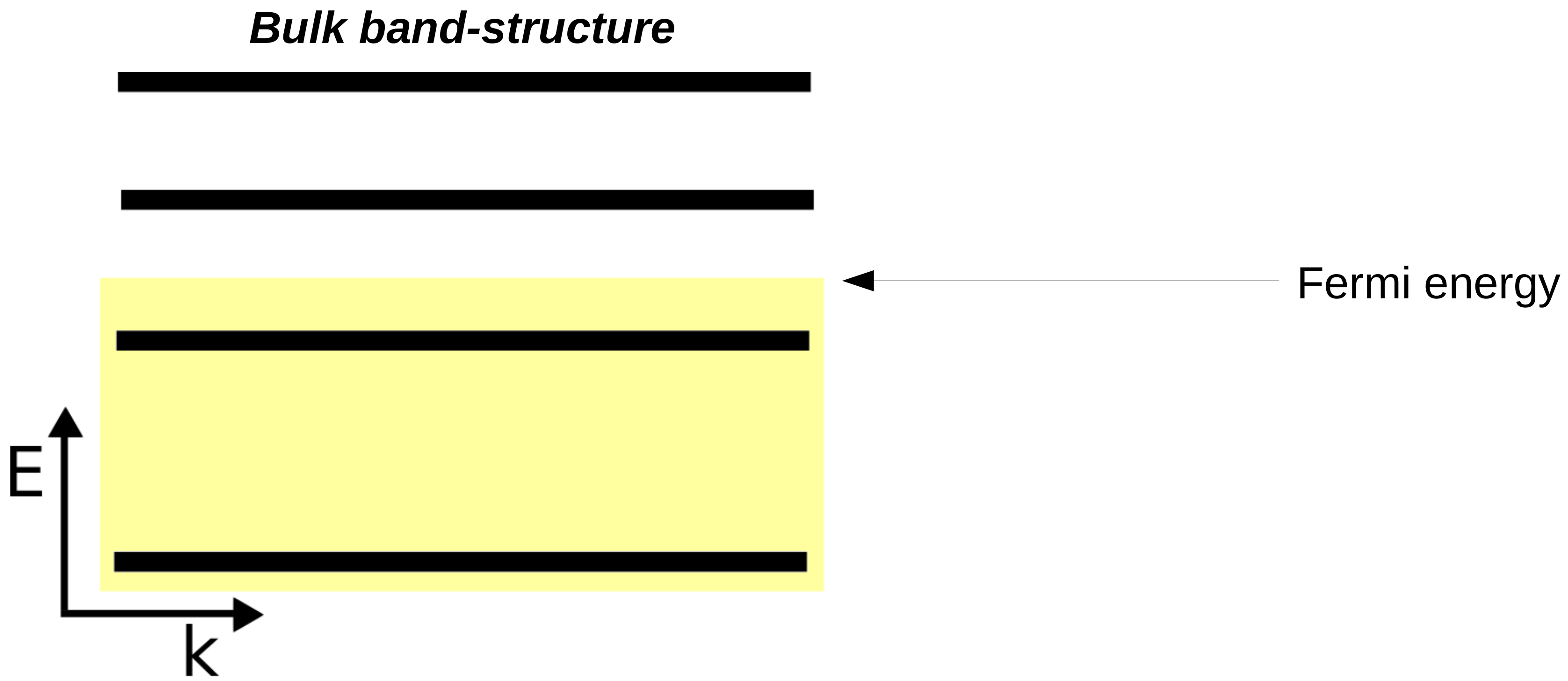
$$\Omega_\alpha = \partial_{k_x} A_y^\alpha - \partial_{k_y} A_x^\alpha$$

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

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

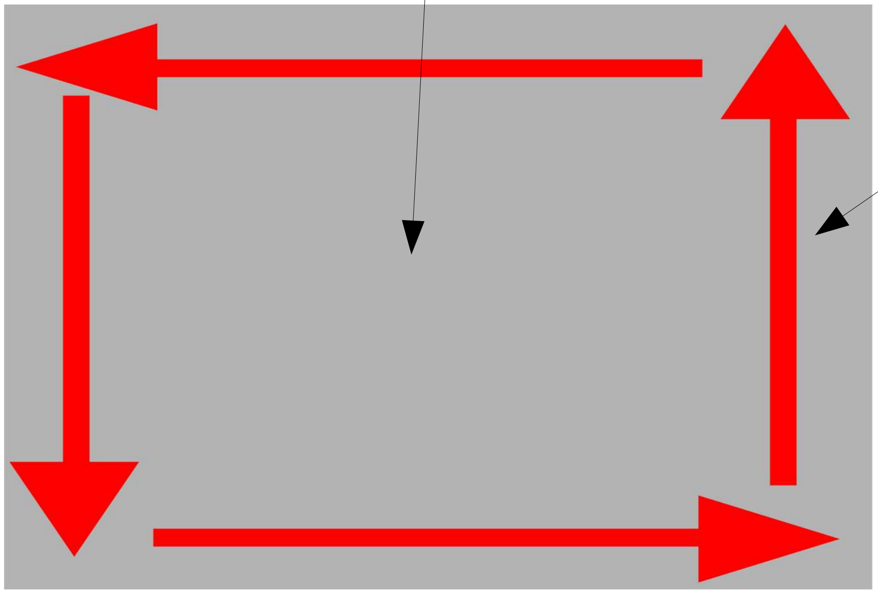
The quantum Hall effect

How can an insulator have conductivity?



The quantum Hall effect

The bulk of a quantum Hall state is insulating



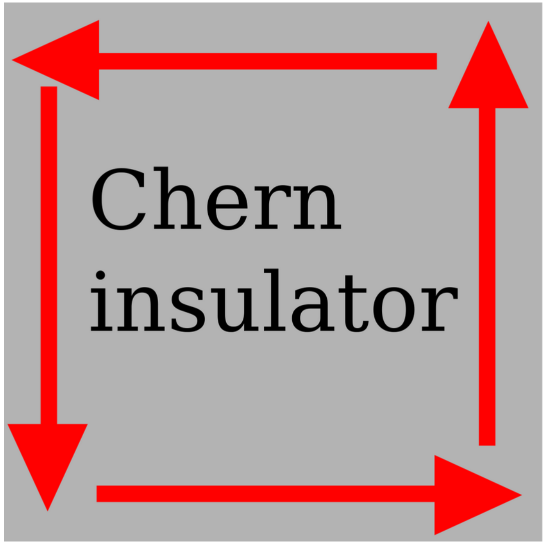
The edge has chiral states

Chiral: propagating only in one direction

Hall conductivity in an insulator

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

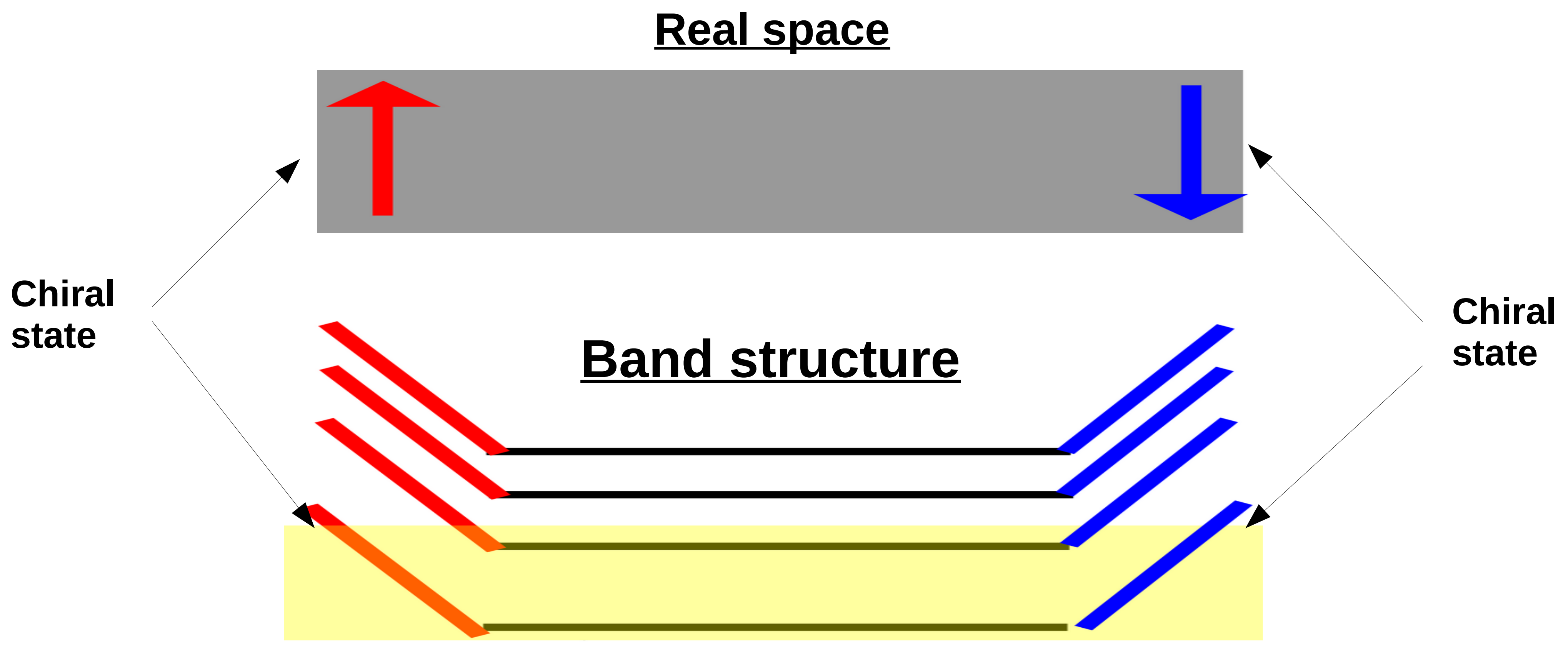
The Chern number for each band is quantized $C_\alpha = \int \Omega_\alpha(\mathbf{k}) d^2\mathbf{k} = 0, \pm 1, \pm 2, ...$



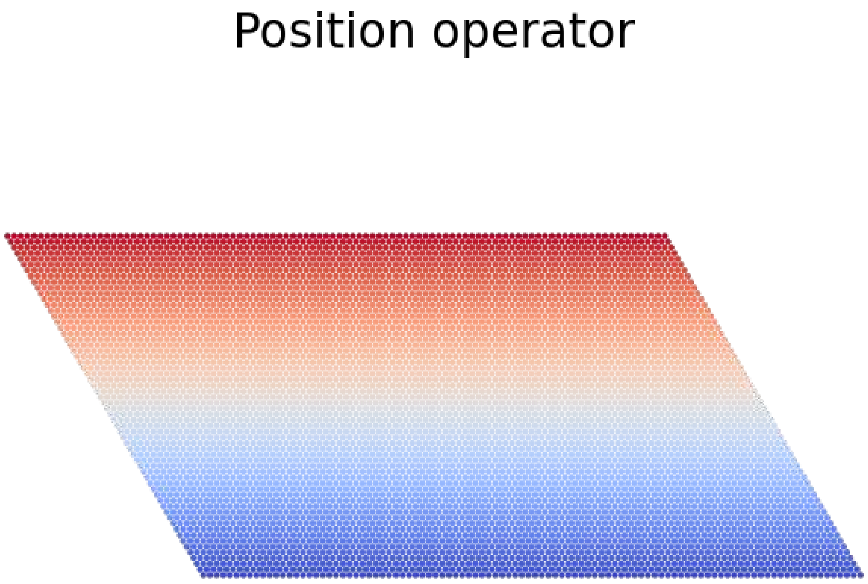
An insulator can have a finite (and quantized) Hall conductivity

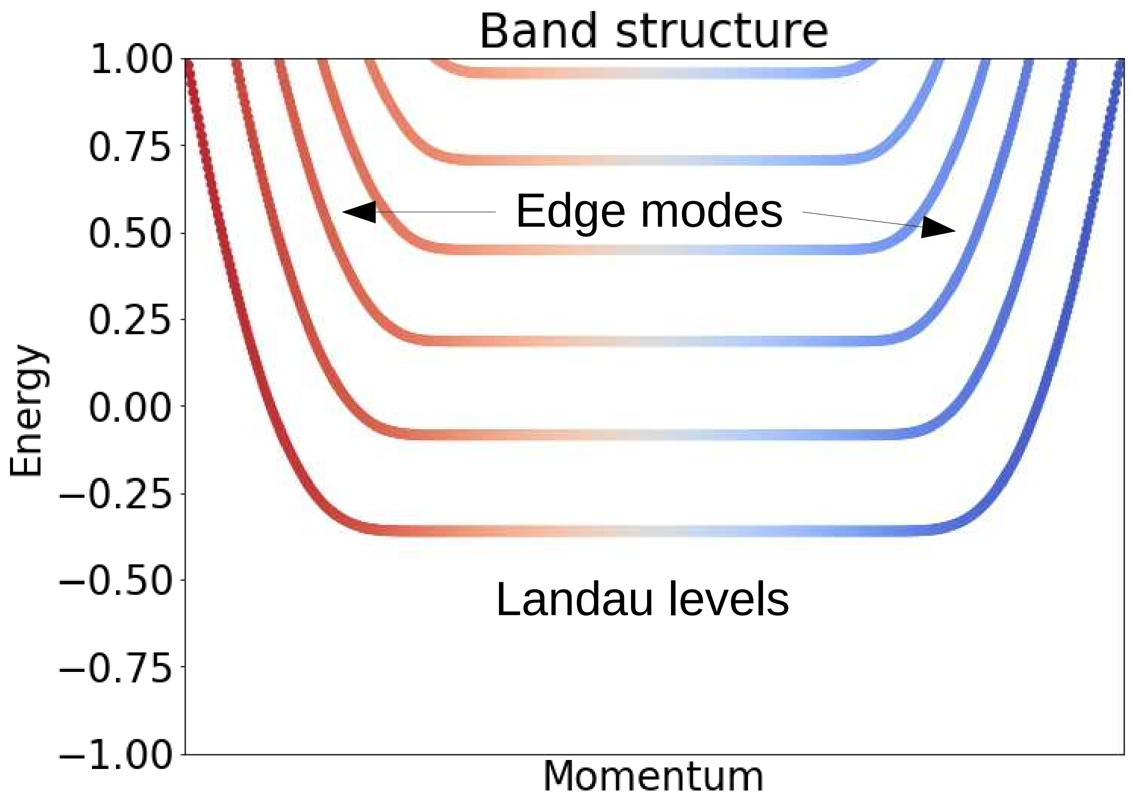
This is a simple example of a topological state of matter

The quantum Hall effect



The quantum Hall effect in a 2D TMDC





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

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

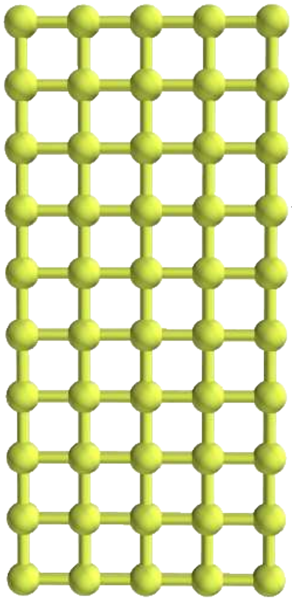
Leading (in the Landau gauge) to the Hamiltonian

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

Quantum Hall effect and quasiperiodicity

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

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



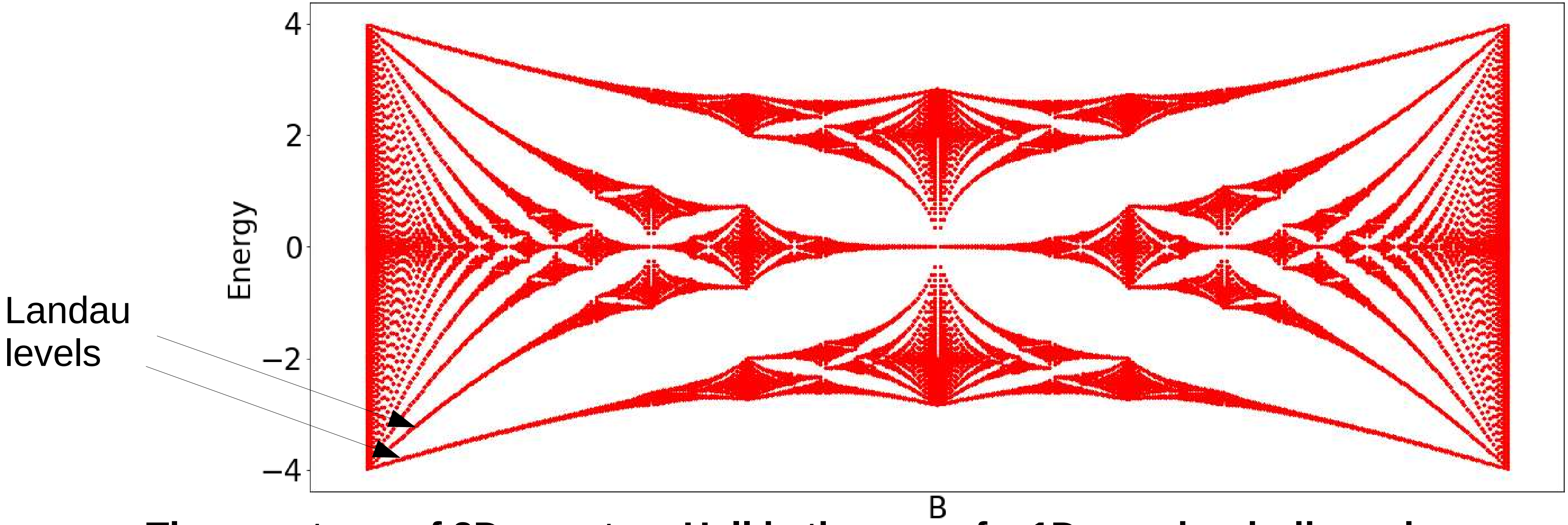
Fourier transform in the infinite direction

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

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 moire

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

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

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

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

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

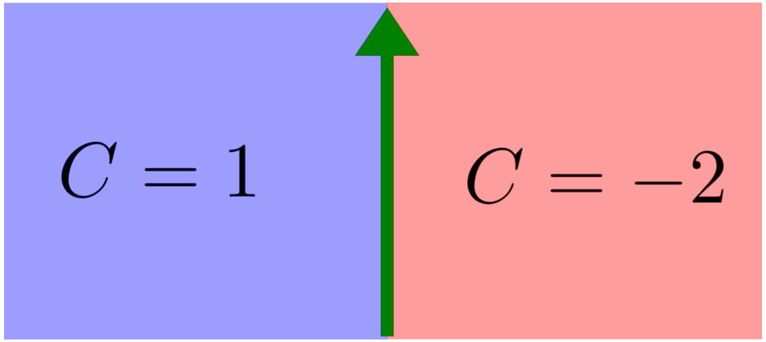
Peierls substitution

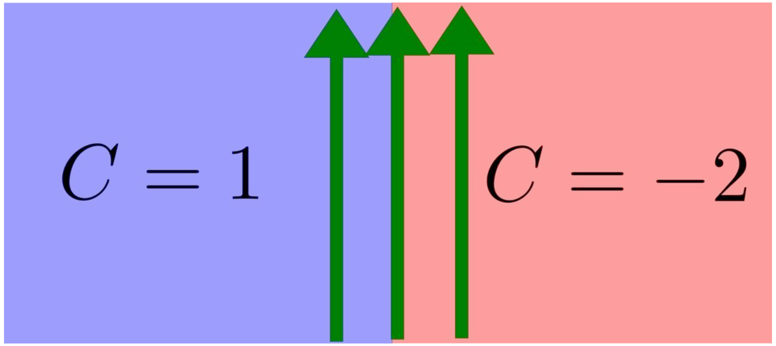
Break

10-15 min break

(optional) to discuss during the break

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

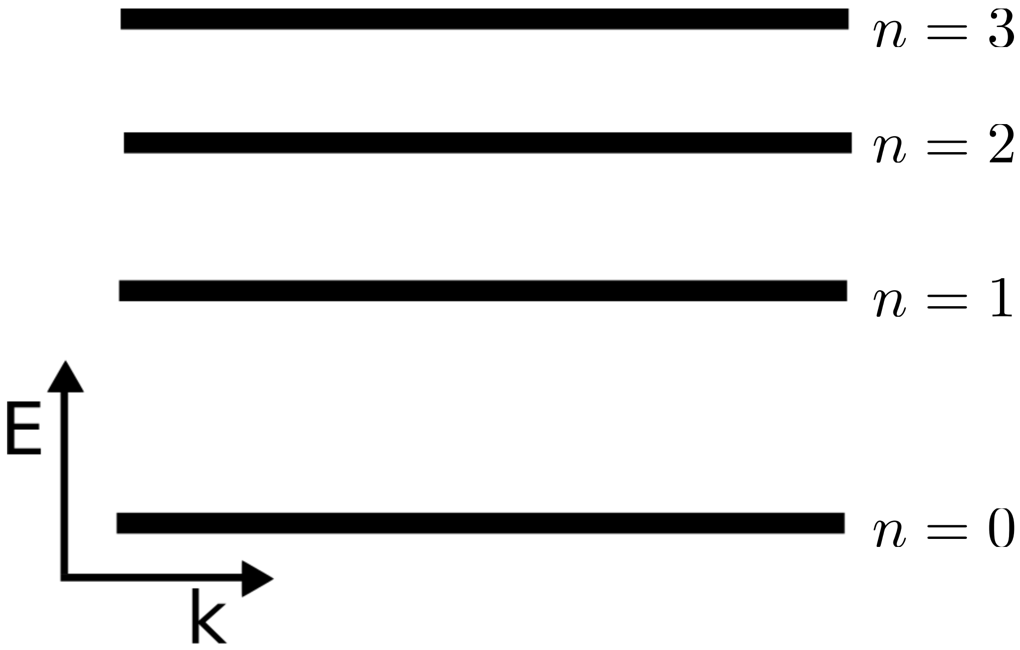




Landau levels

Landau levels

Band-structure in the quantum Hall state



The energy levels are

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

$$E \sim 1meV$$

For a Dirac equation they would be

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

$$E \sim 50meV$$

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) $$\mathbf{p} \to \mathbf{p} + \mathbf{A}$$

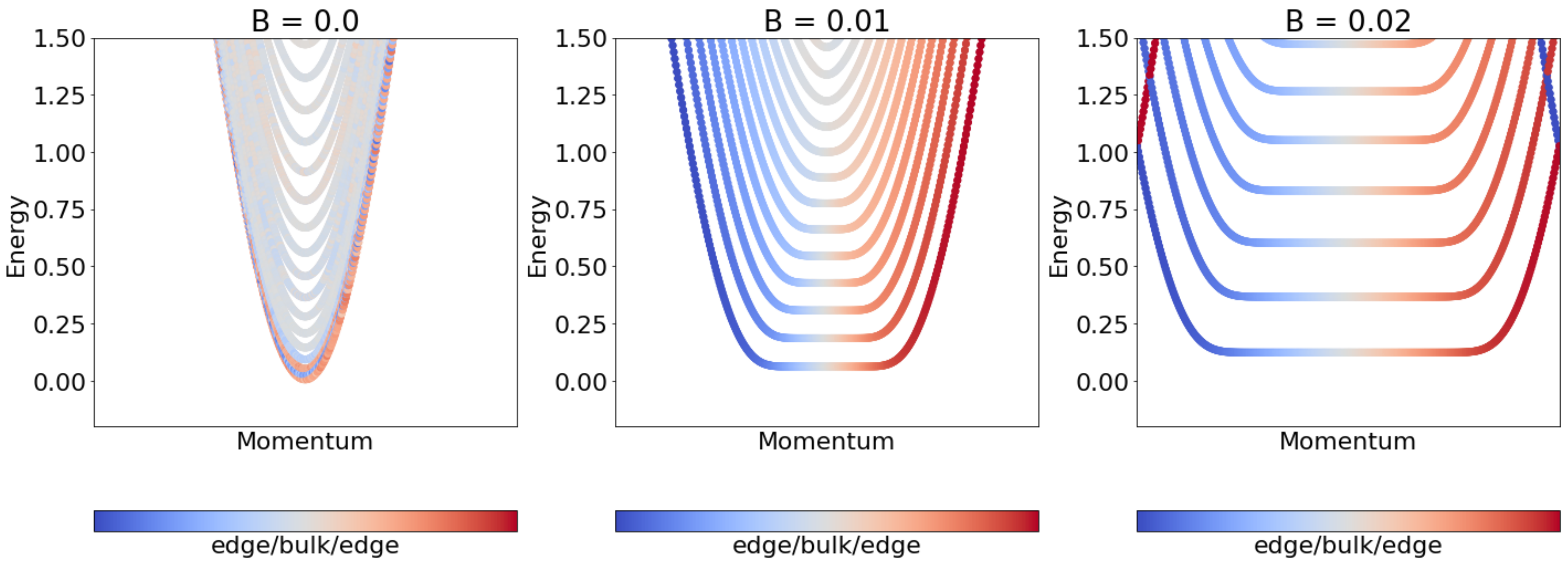
Take the Landau gauge
$$\mathbf{A} = (0, -Bx, 0)$$
$$\nabla \times \mathbf{A} = (0, 0, B)$$

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 $$E_n \sim nB$$

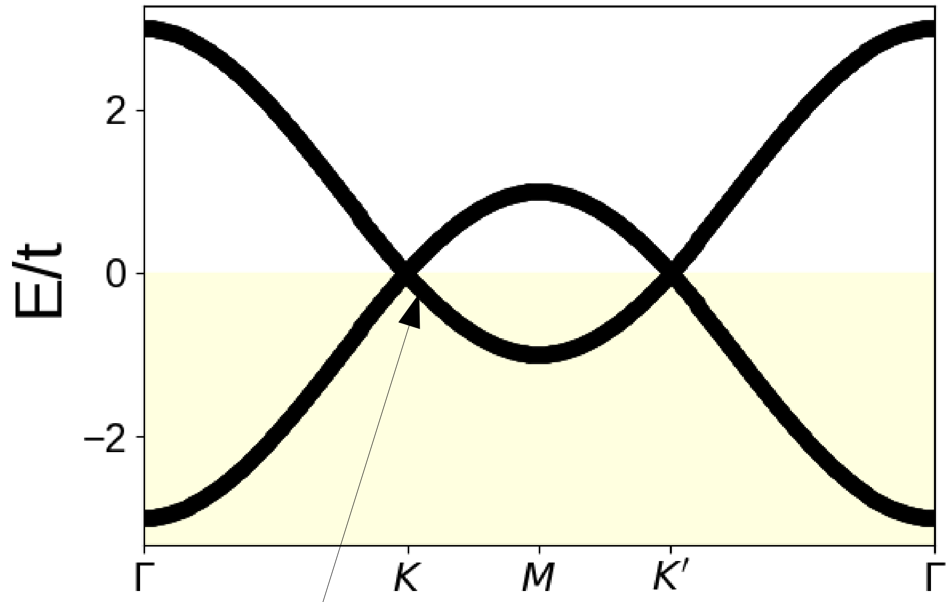
Landau levels of a 2D TMDC



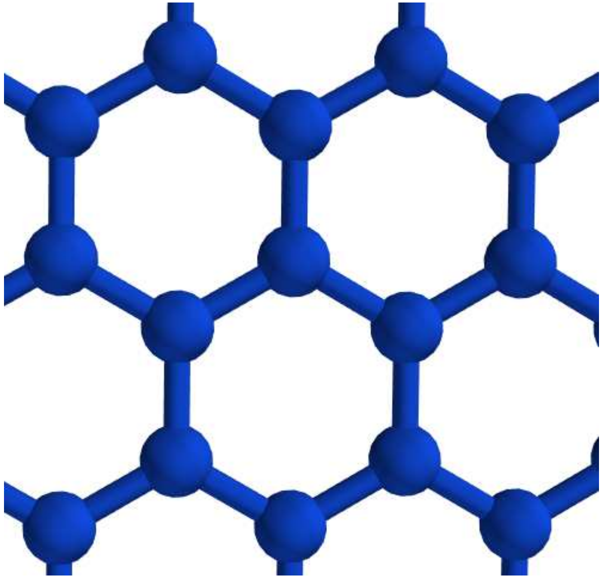
As the magnetic field is increased, flat band Landau levels appear

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

$$H^2 \sim p_x^2 + B^2 x^2$$

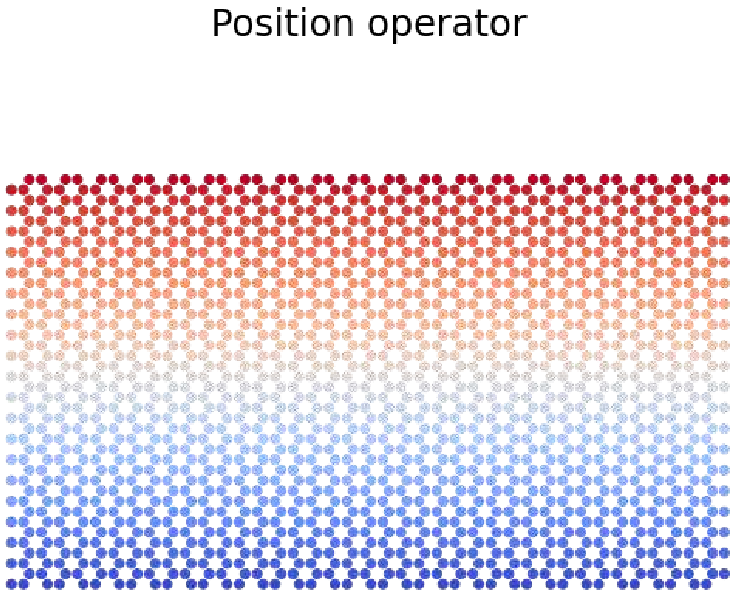
(this looks like an harmonic oscillator)

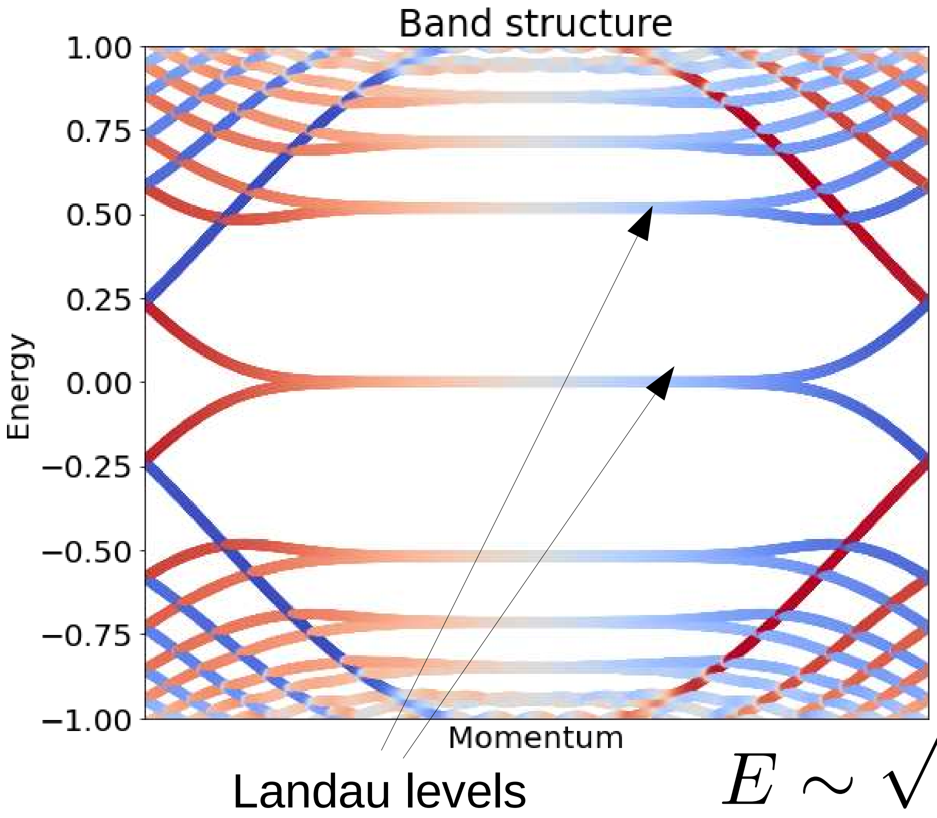
$$E_n^2 \sim nB$$

Quantized levels in a magnetic field

$$E_n \sim \sqrt{nB}$$

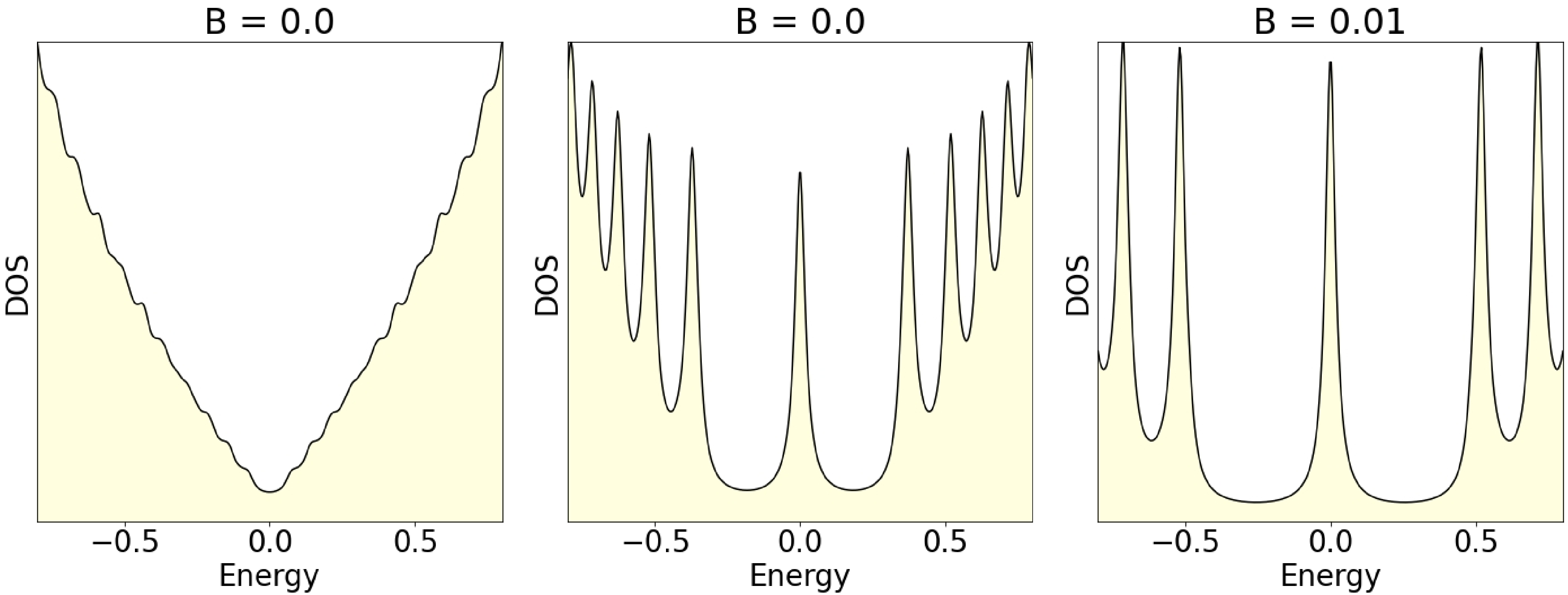
The Landau levels in graphene





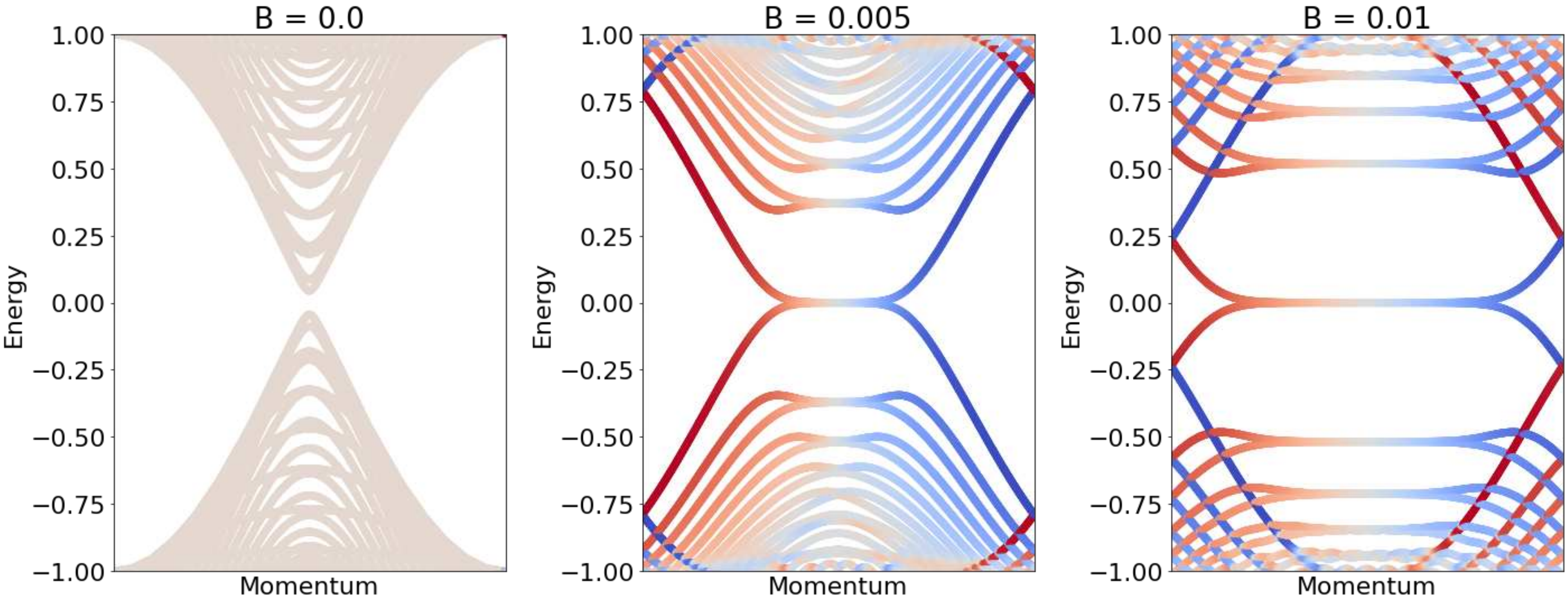
$$E \sim \sqrt{nB}$$

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



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

The zeroth Landau level in graphene

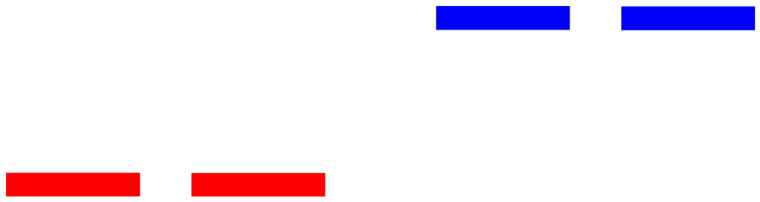
In the Dirac equation, each valley contributed with one Landau level at E=0

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

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

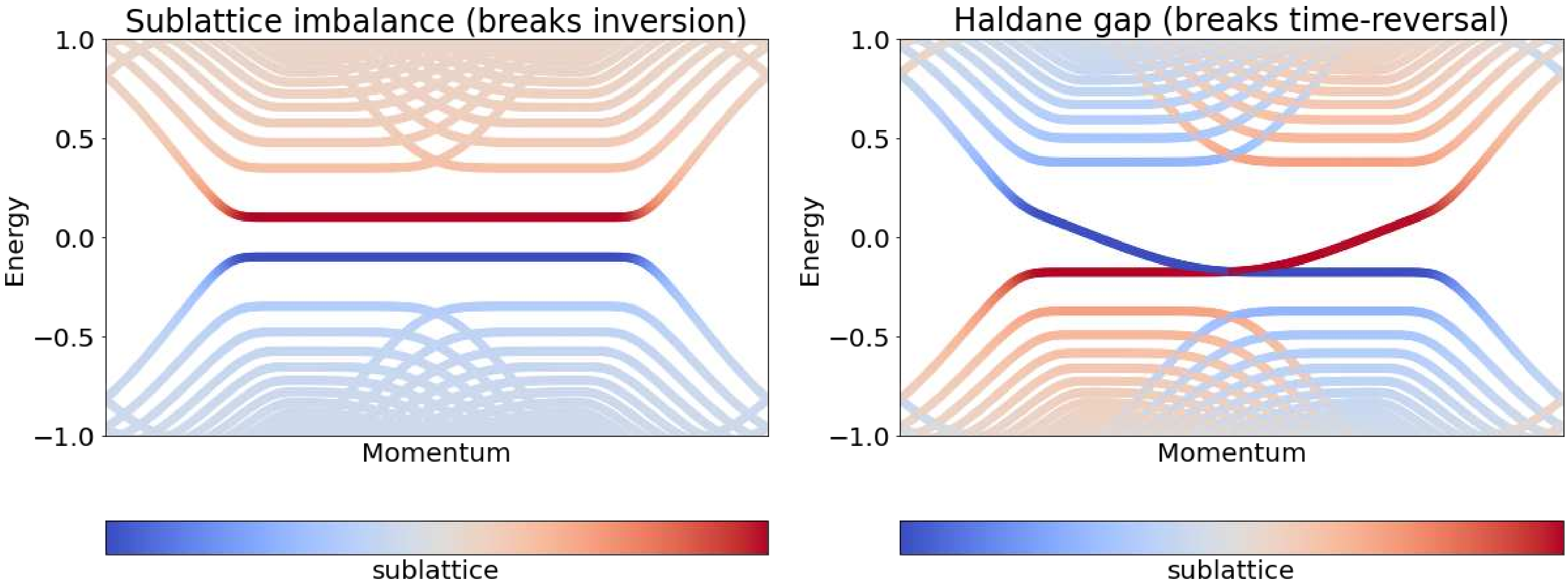
In the absence of symmetry breaking

In the presence of symmetry breaking



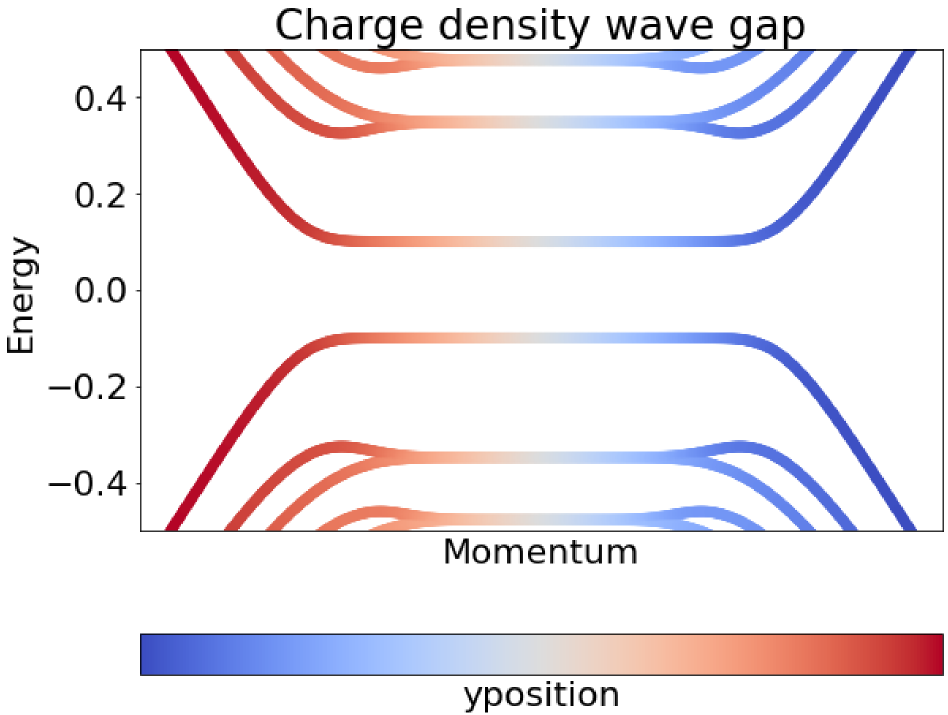
Symmetry breaking the zeroth Landau level gives rise to different topological states

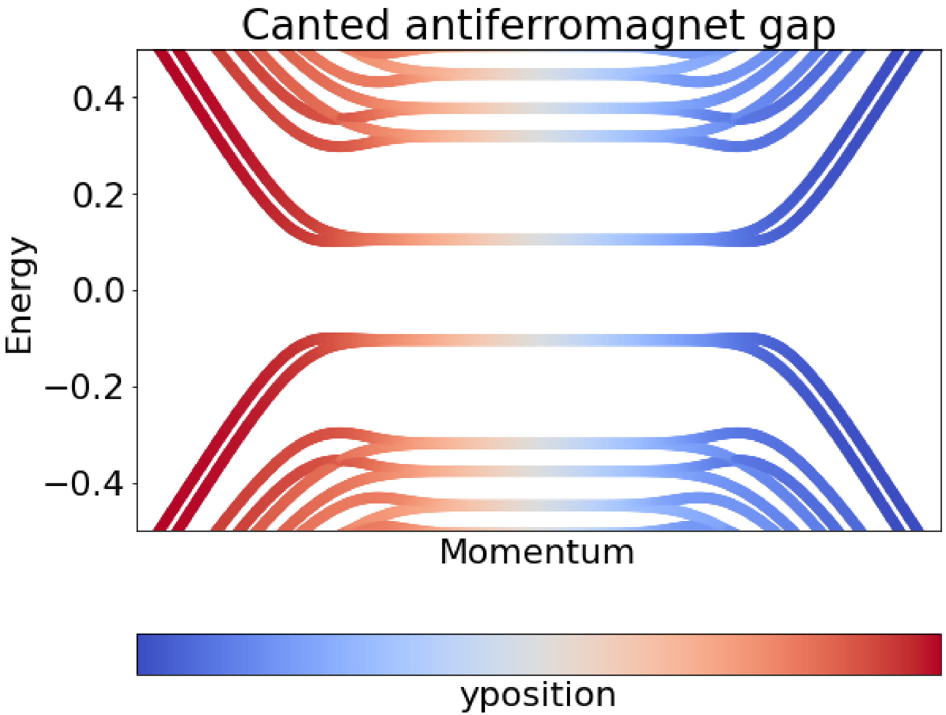
The zeroth Landau level in graphene



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

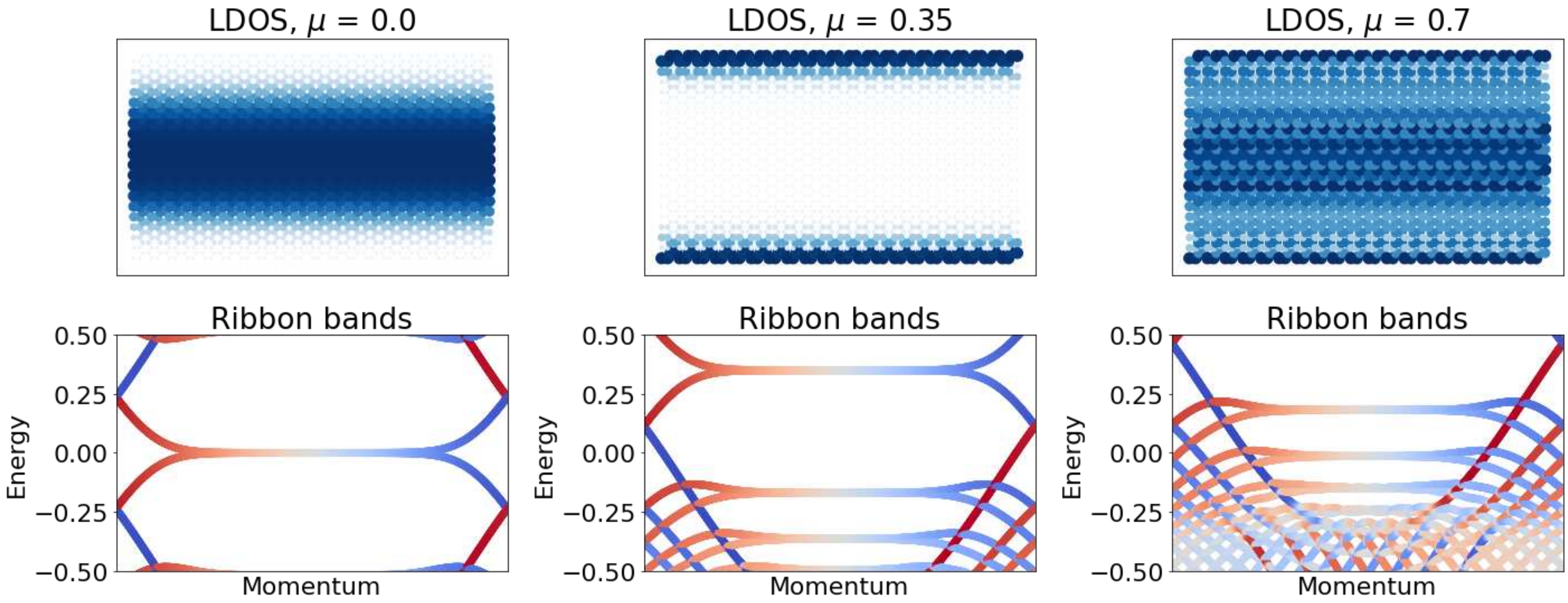




Both CDW and canted antiferromagnetism lead to gapped system without edge modes

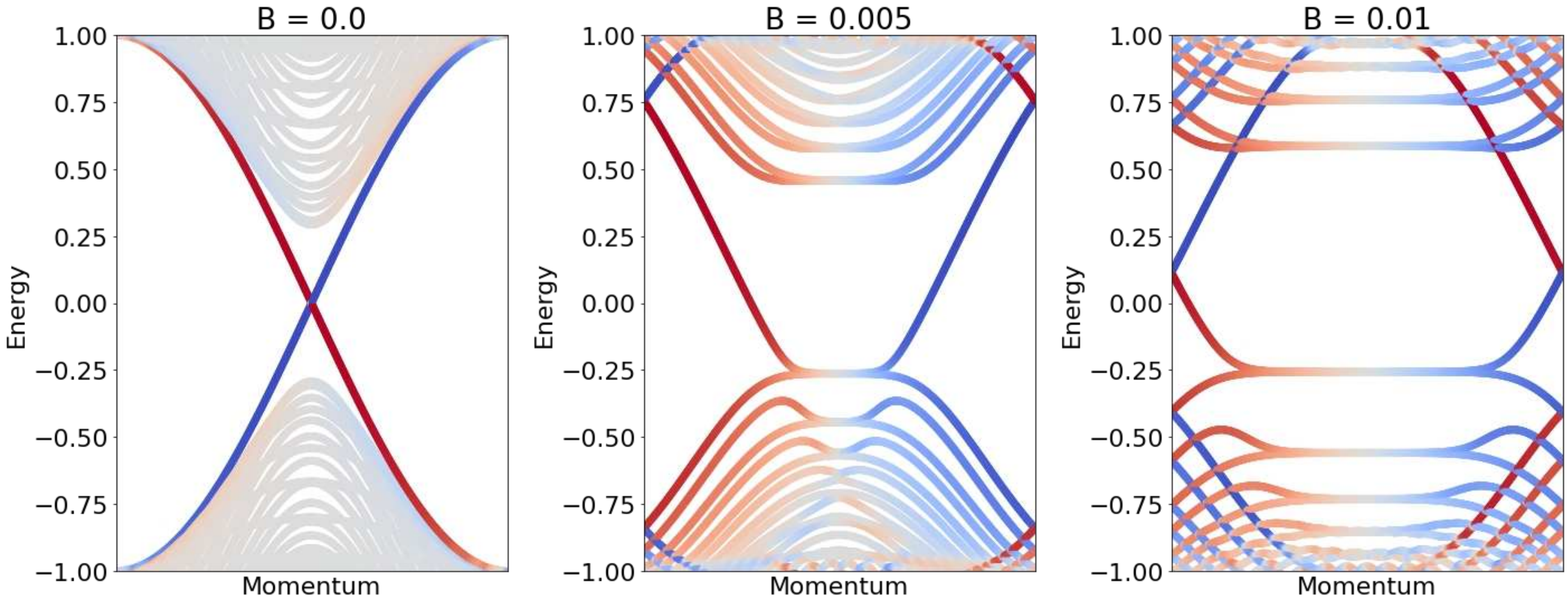
Location of the edge states in the quantum Hall state in graphene

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



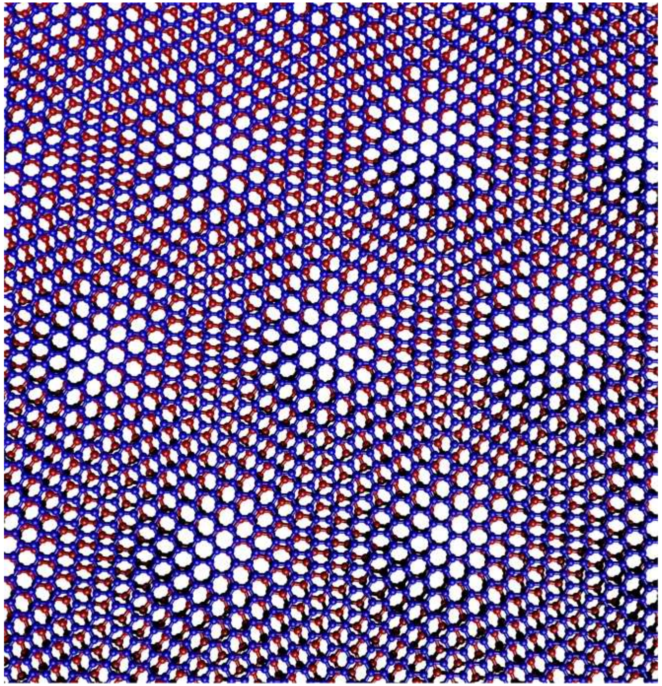
States between LL are located at the edge, while LL are located in the bulk

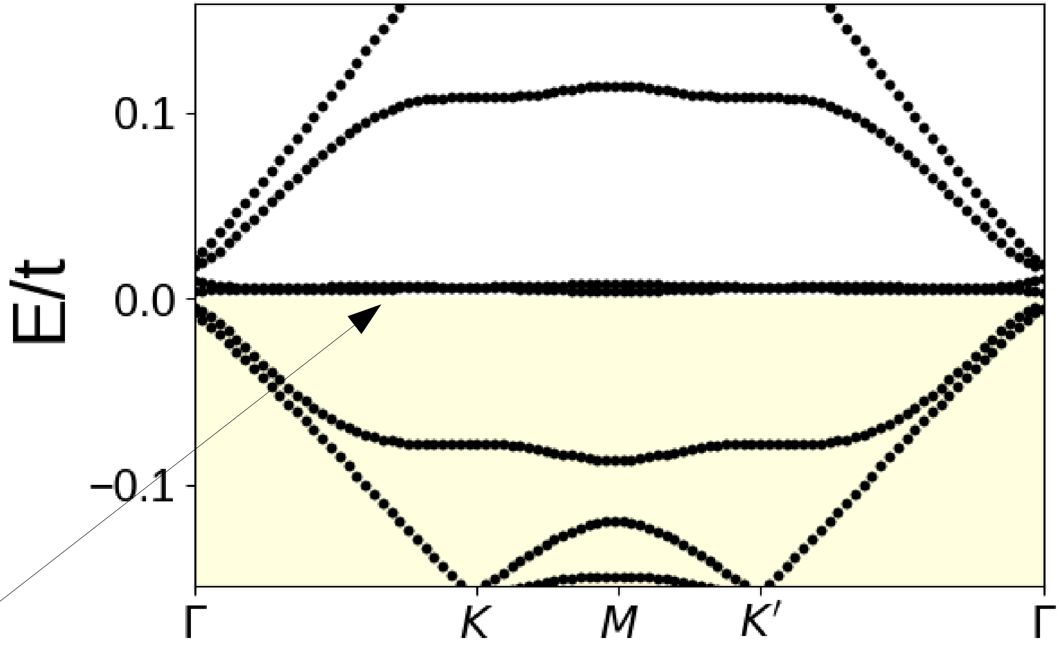
From a Chern insulator to a quantum Hall state



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

Chern insulators in twisted graphene bilayers

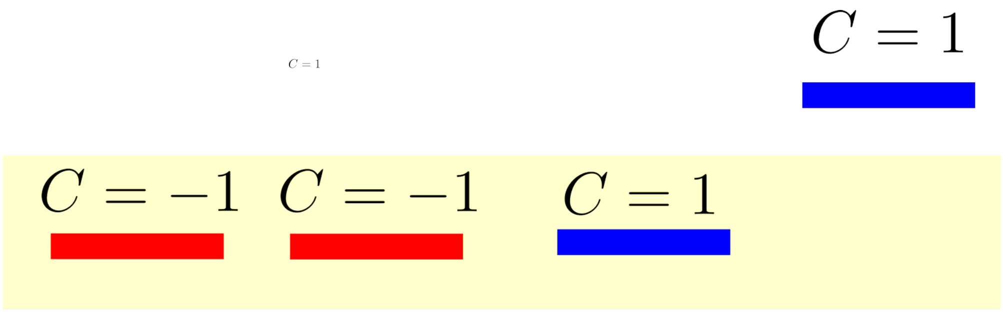


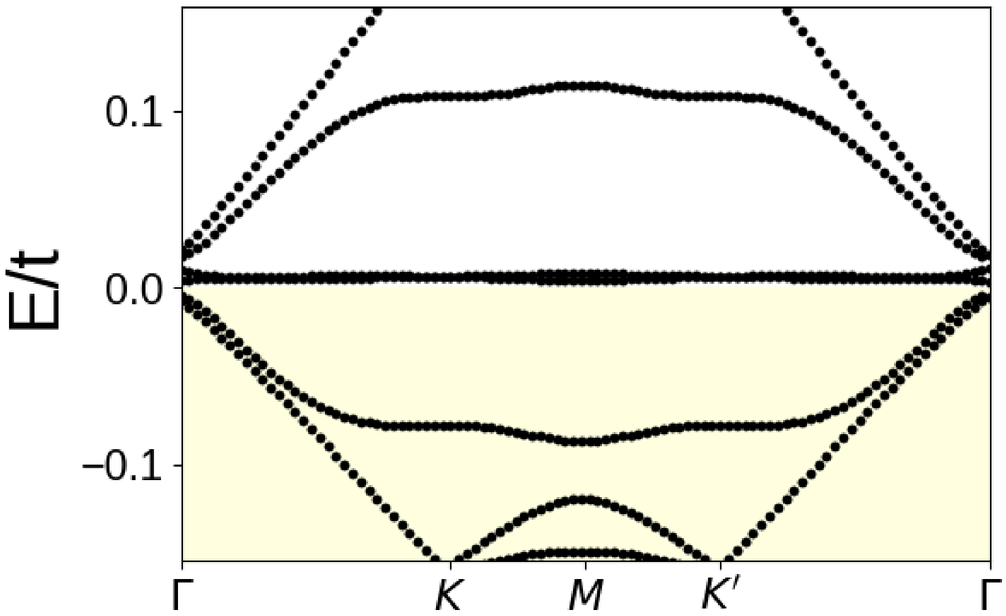


The flat bands of twisted bilayers are pseudo Landau levels

Chern insulators in twisted graphene bilayers

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



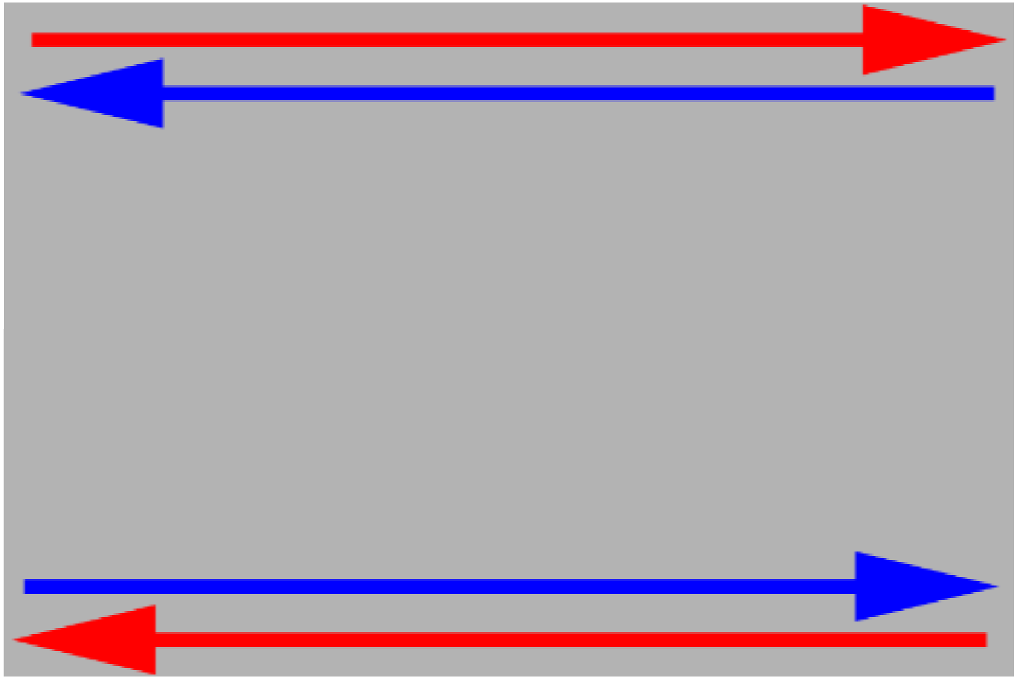


hBN encapsulation allows to lift the Dirac points

Van der Waals quantum spin Hall insulators

Edge states in quantum spin Hall insulators

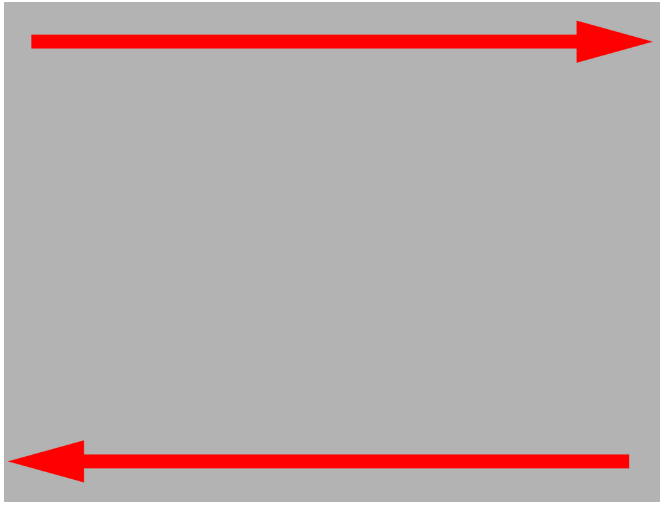
In a quantum spin Hall insulator, opposite spin propagate in opposite directions



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

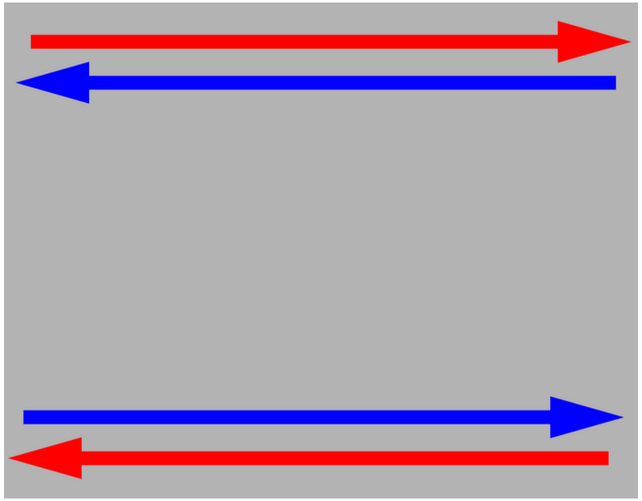
The relation between two topological states

Chern insulators



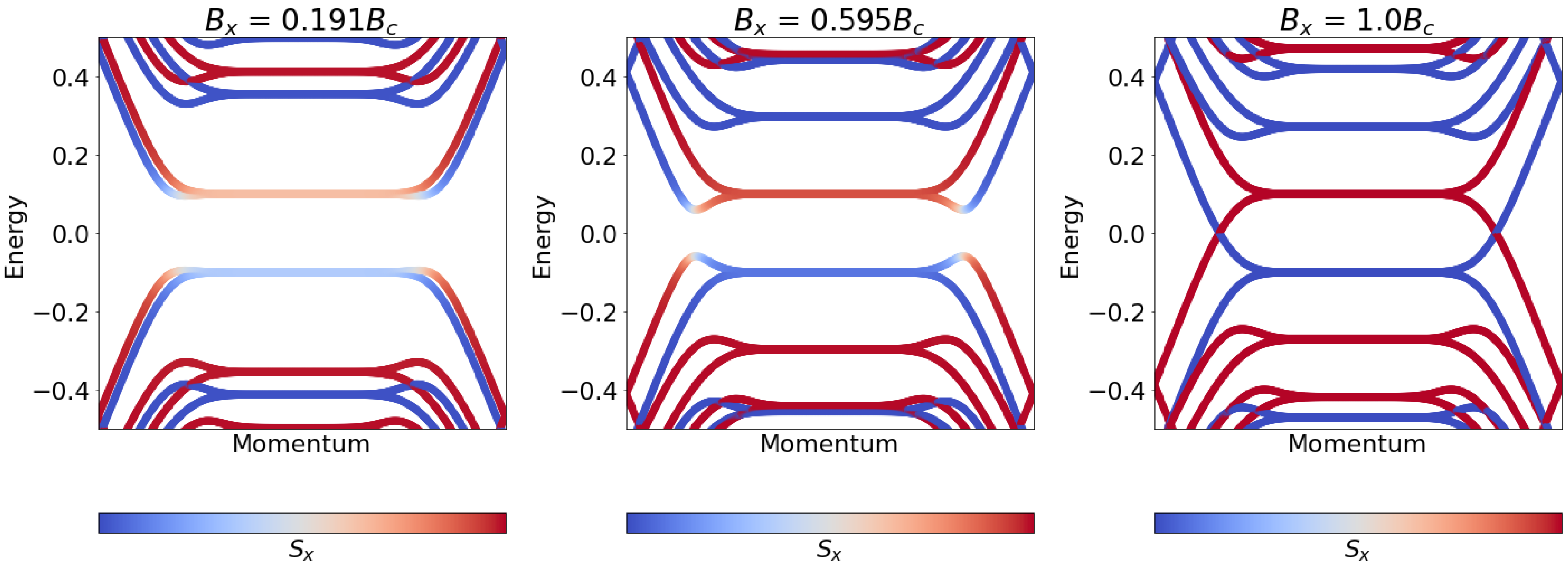
Chiral modes
Break time-reversal symmetry

Quantum spin Hall insulators



Helical modes
Do not break time-reversal symmetry

The quantum spin Hall state driven by magnetic field in graphene

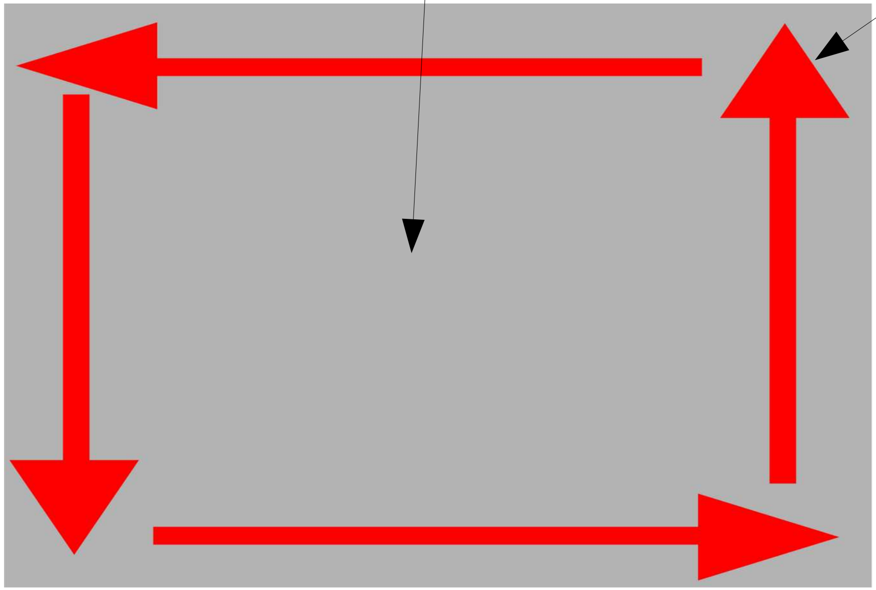


As an in-plane field in increased, a trivial QH state transforms in a quantum spin Hall state

Chern insulators

The bulk is insulating

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



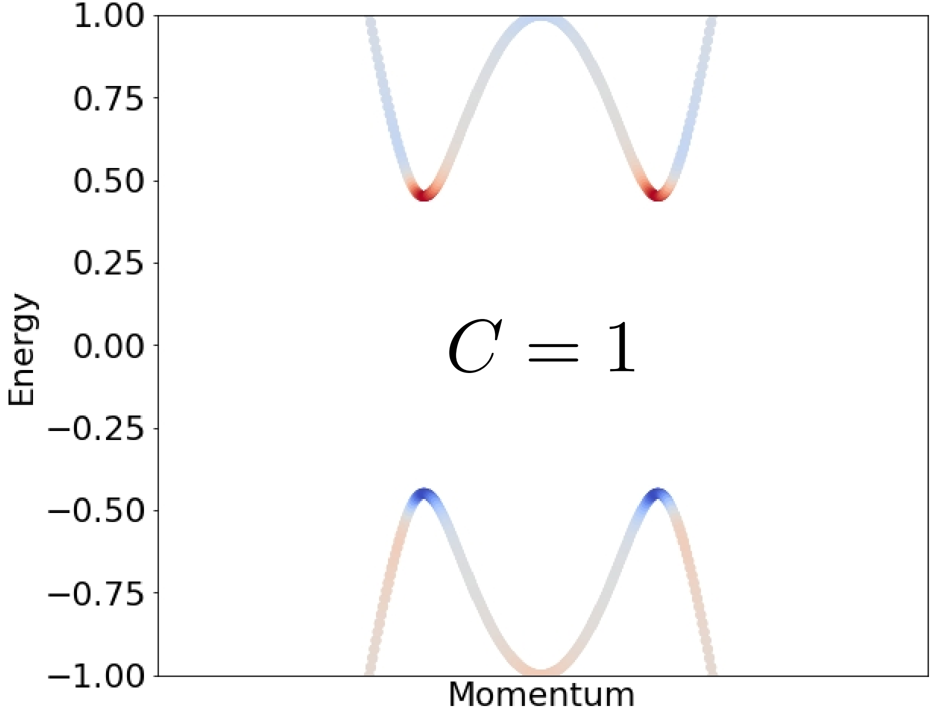
Hall conductivity (Chern number)

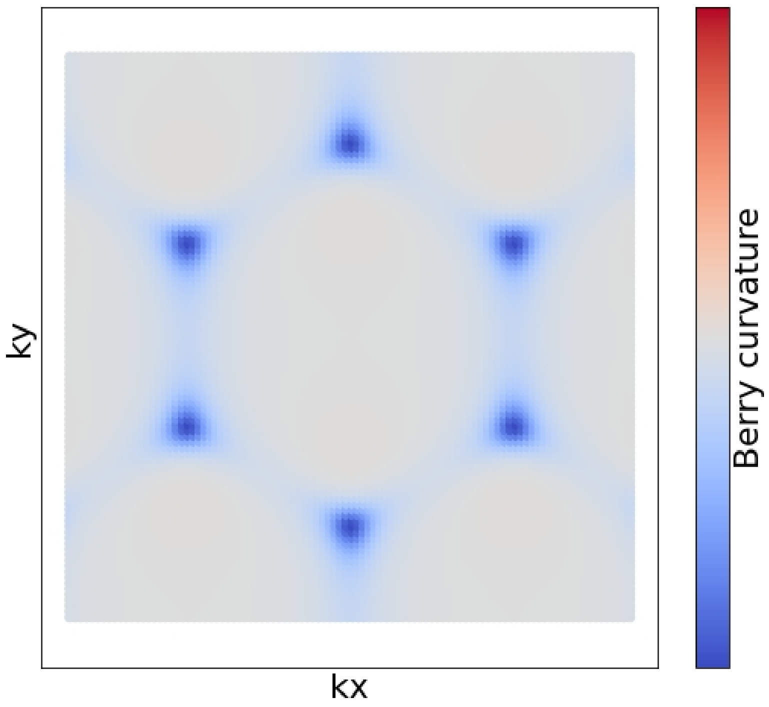
$$\sigma_{xy} = \sum_{\alpha \in occ} \int \Omega_\alpha d^2\mathbf{k} = \sum_\alpha C_\alpha = C$$

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

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

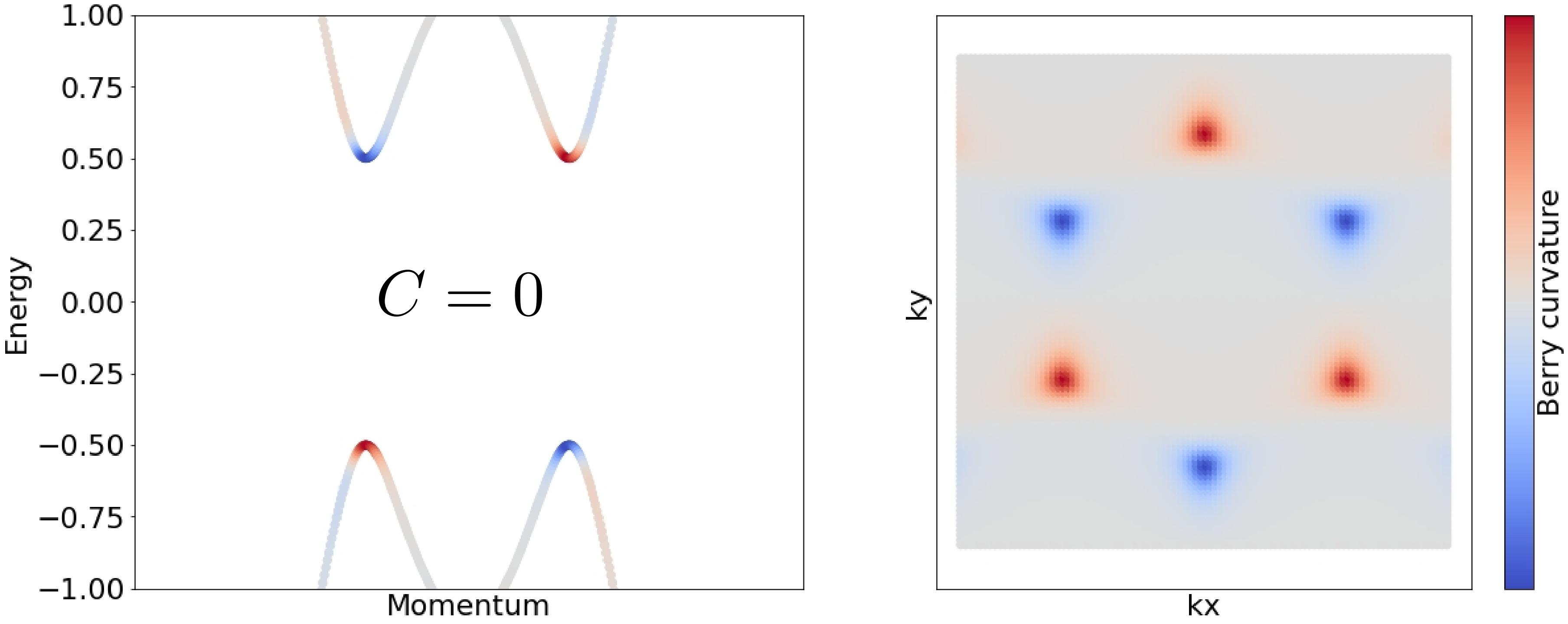
Two different gaps in a 2D material





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 $C_{s,\alpha} = \frac{1}{2}\mathrm{sign}(m)\mathrm{sign}(\kappa)$

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

Chern number

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

Spin Chern number

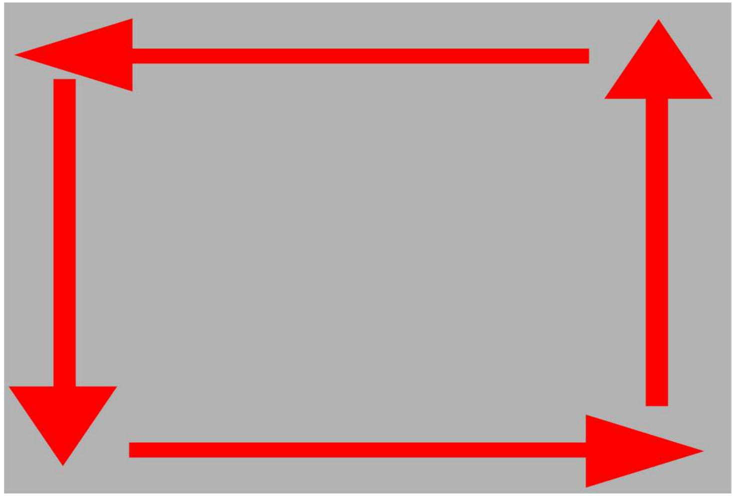
$$C_S = C_\uparrow - C_\downarrow = \pm 2$$

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

Quantum spin Hall insulators

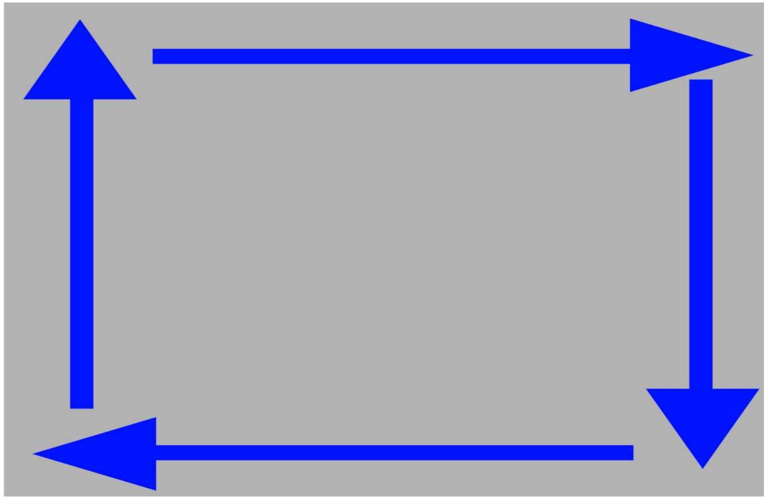
Chern insulator for spin up

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



Chern insulator for spin down

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



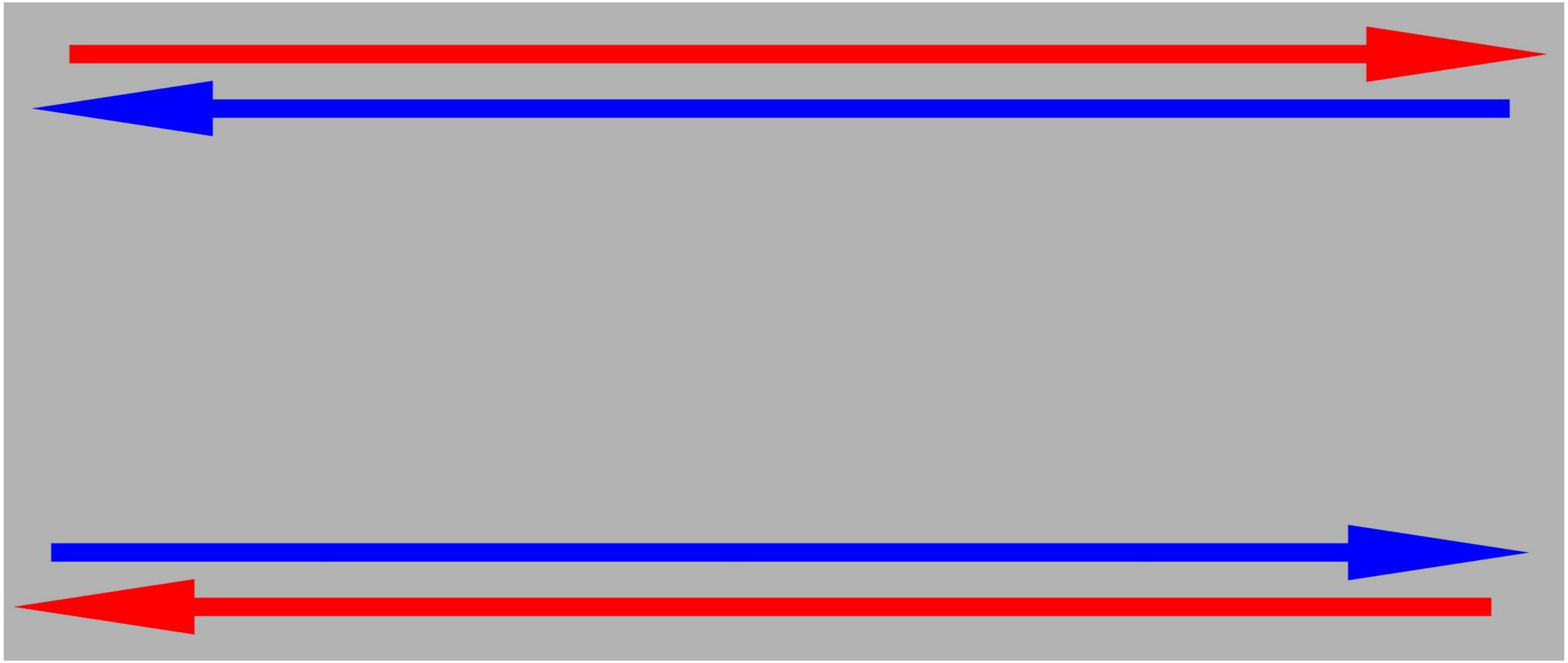
Spin-orbit coupling (SOC) can drive a quantum spin Hall state

$$\vec{L} \cdot \vec{S} \sim L_z S_z$$

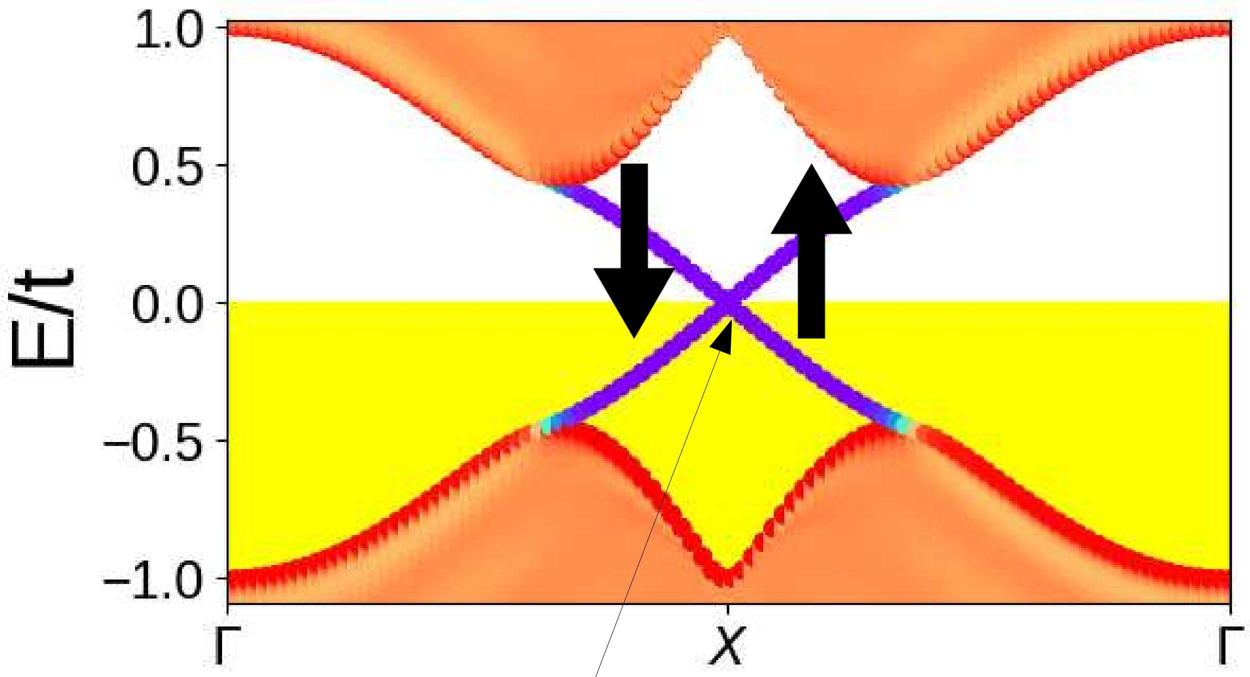
SOC acts as a magnetic field with opposite signs for opposite spins

Quantum spin Hall insulators

Opposite spins propagate in opposite directions (helical gas)



Quantum spin Hall insulators



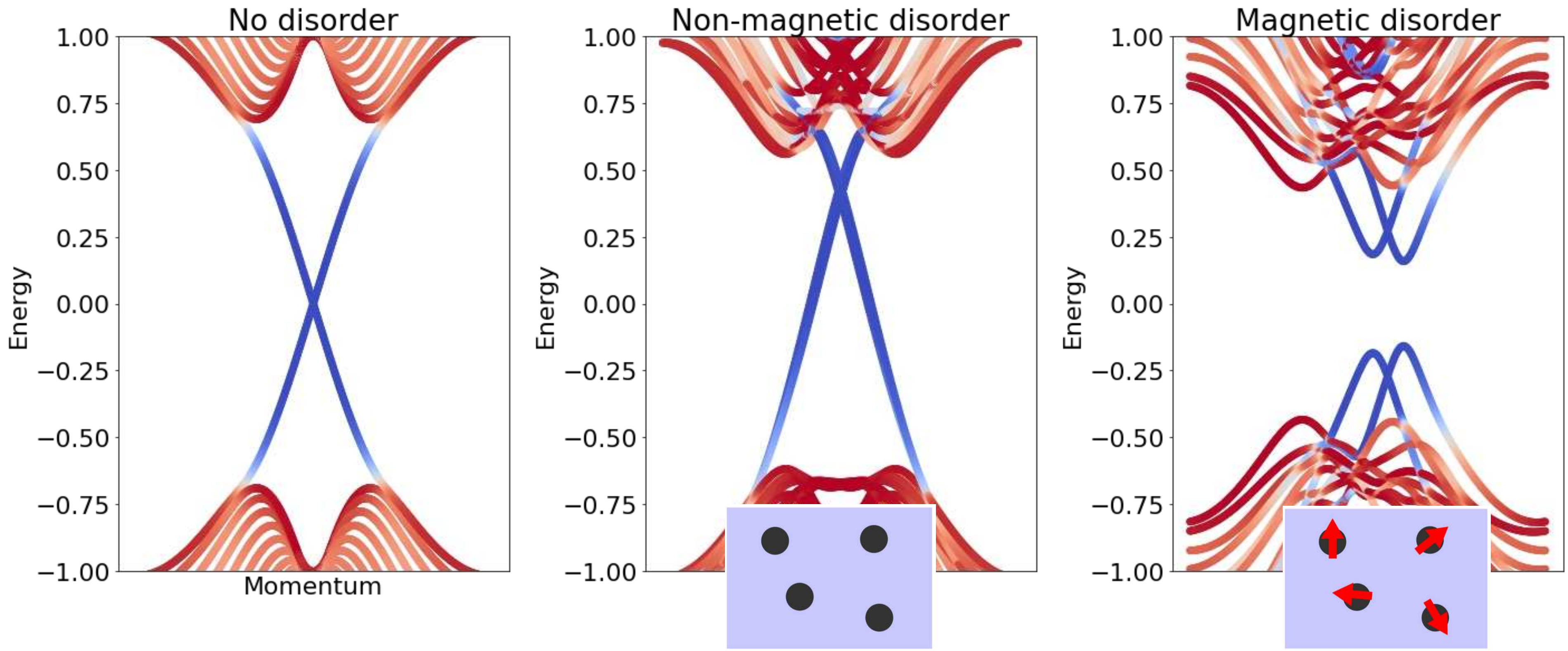
The gapless nature is protected by Kramer’s theorem

1T-WTe$_2$

Time-reversal symmetry

$$\Theta^2 = -1$$

Disorder in quantum spin Hall insulators



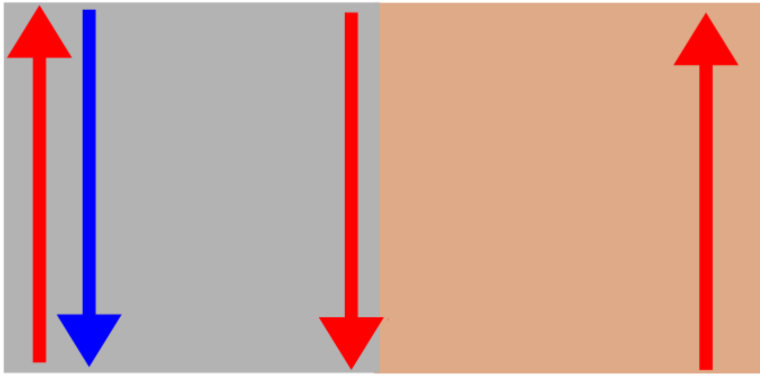
Disorder that breaks time reversal symmetry opens a gap in the topological states

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?



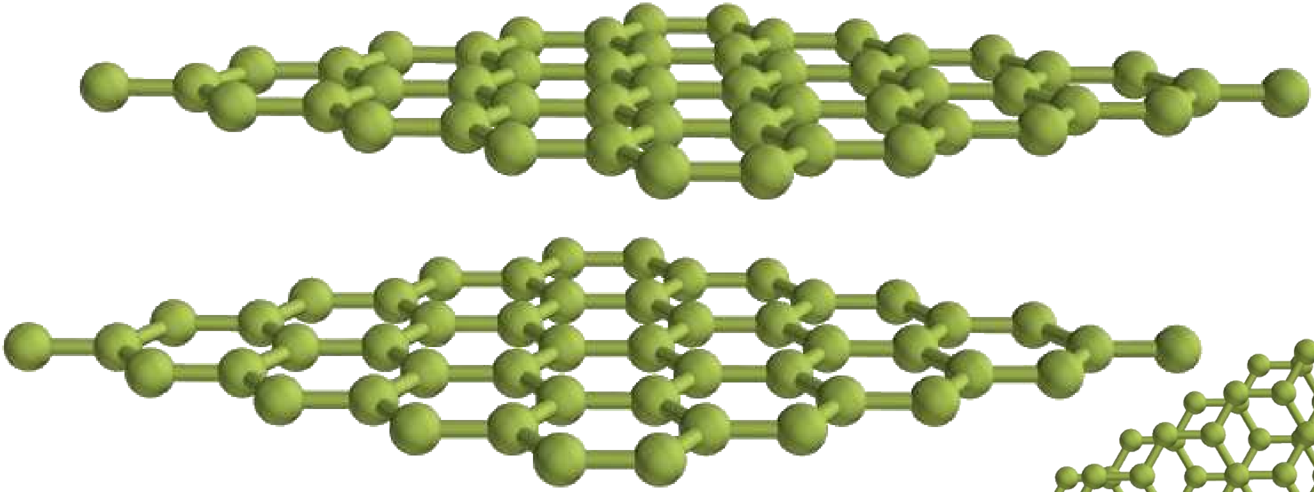
Valley Chern insulators
2D materials

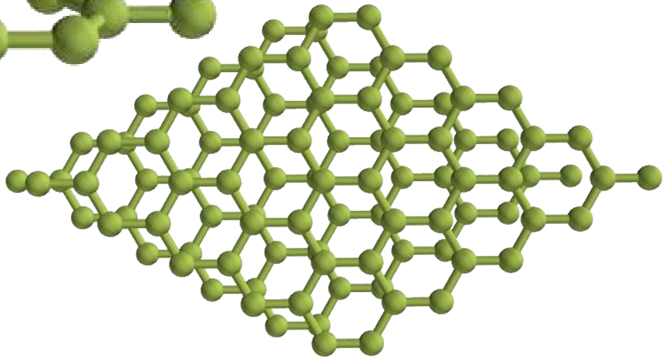
The structure of bilayer graphene

Let us now focus on a graphene bilayer with AB stacking

$$+Ec_n^\dagger c_n$$

$$-Ec_n^\dagger c_n$$

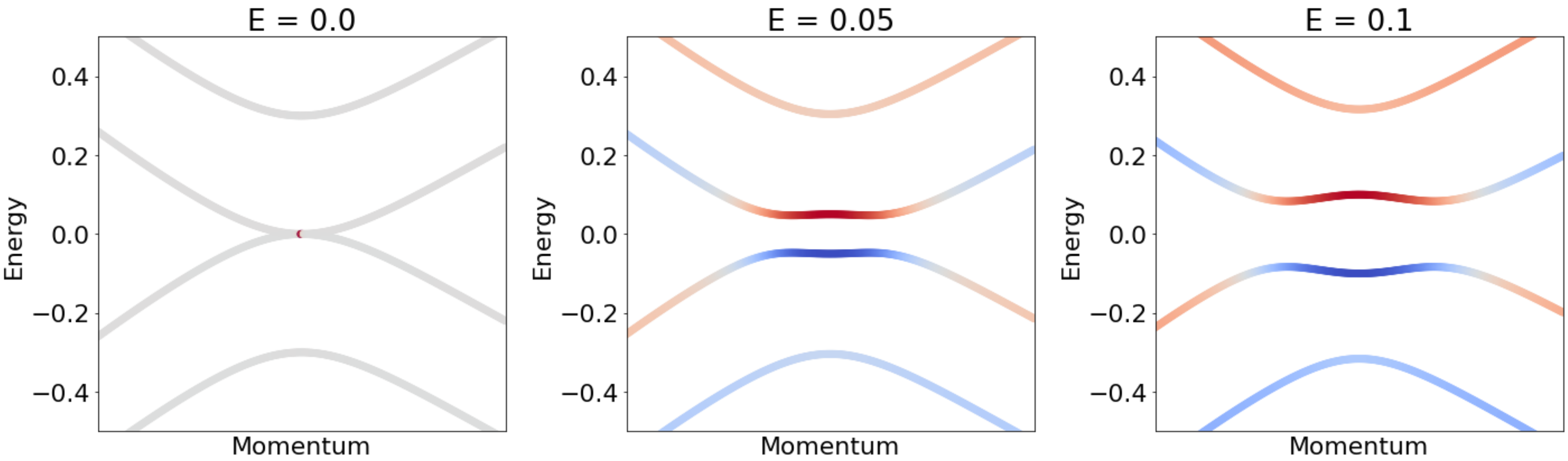




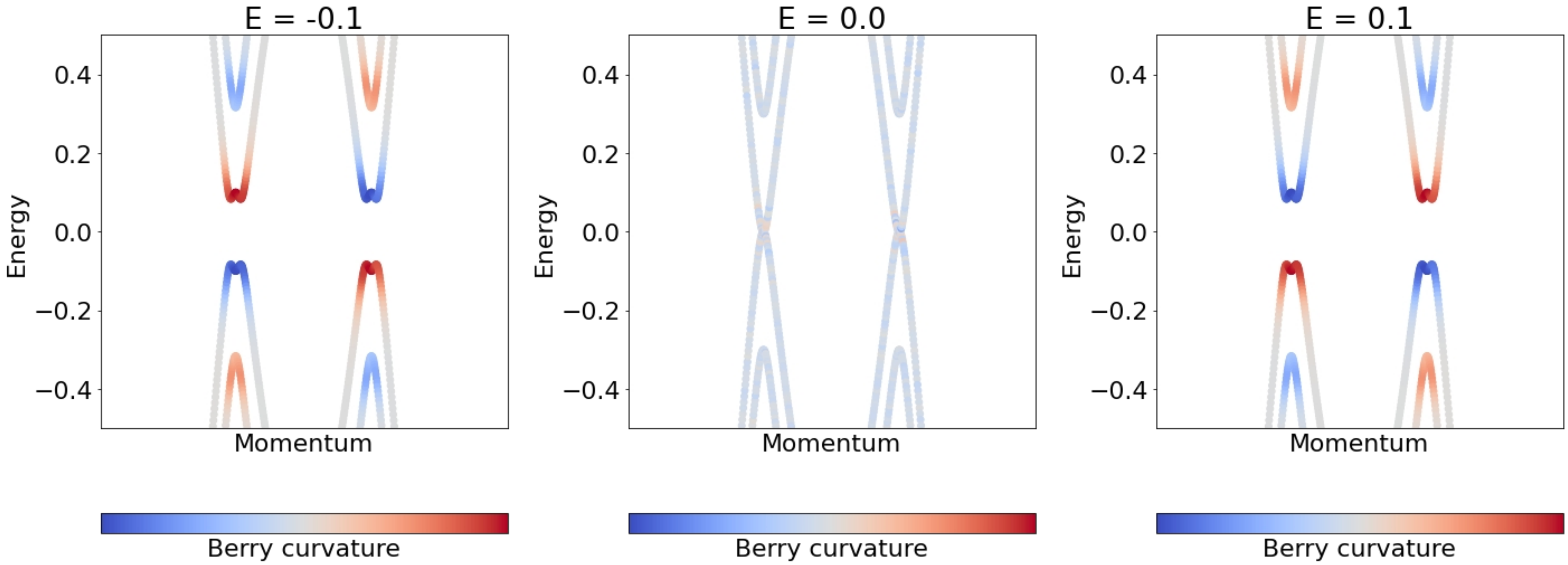
And we will add an interlayer bias

The electronic structure of bilayer graphene

Graphene bilayers open a gap when an interlayer bias is applied

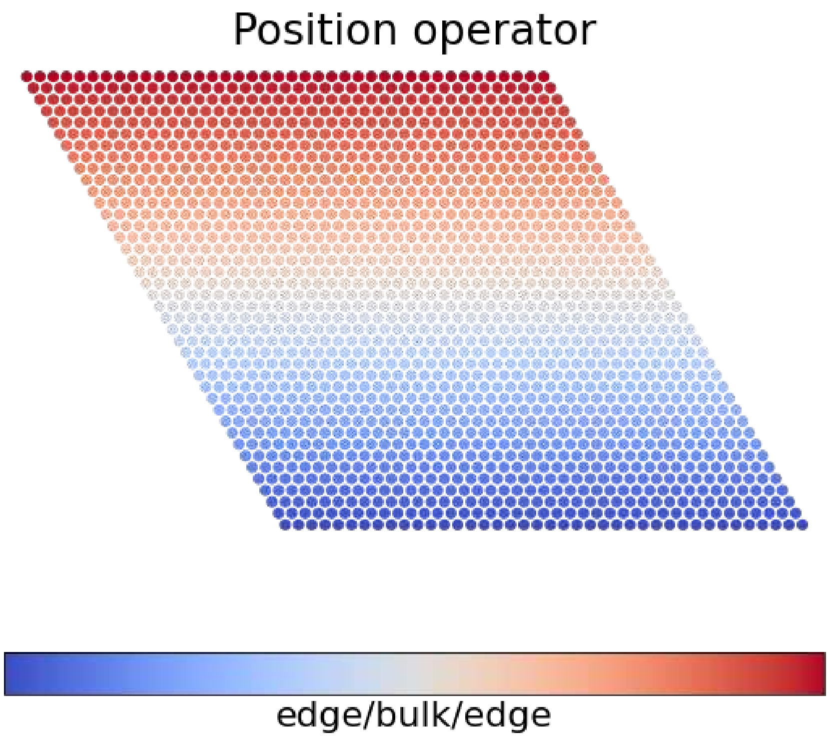


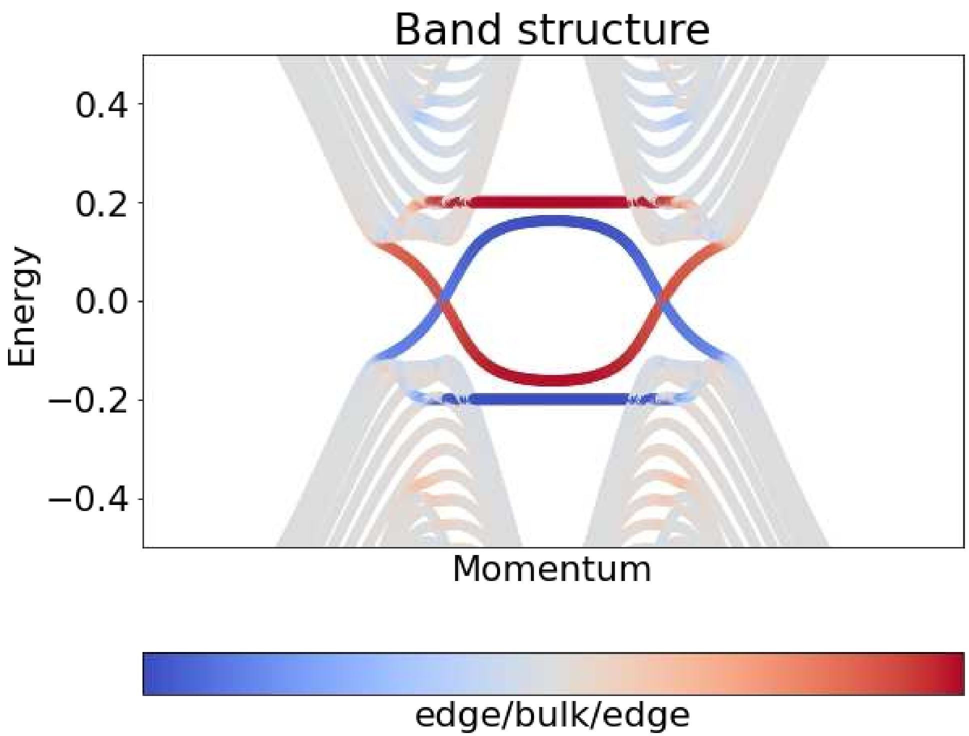
Electrically controllable topology in graphene bilayers



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

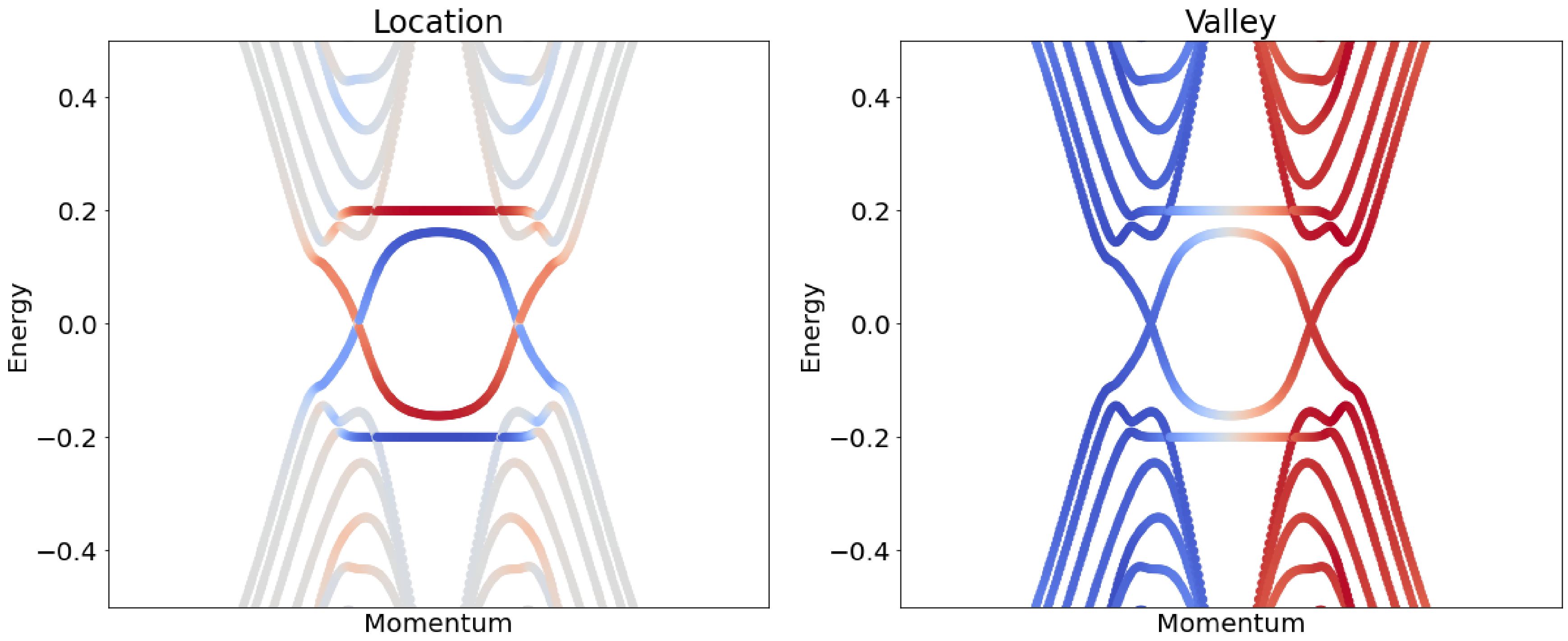
Biased bilayer graphene, pseudo-helical states





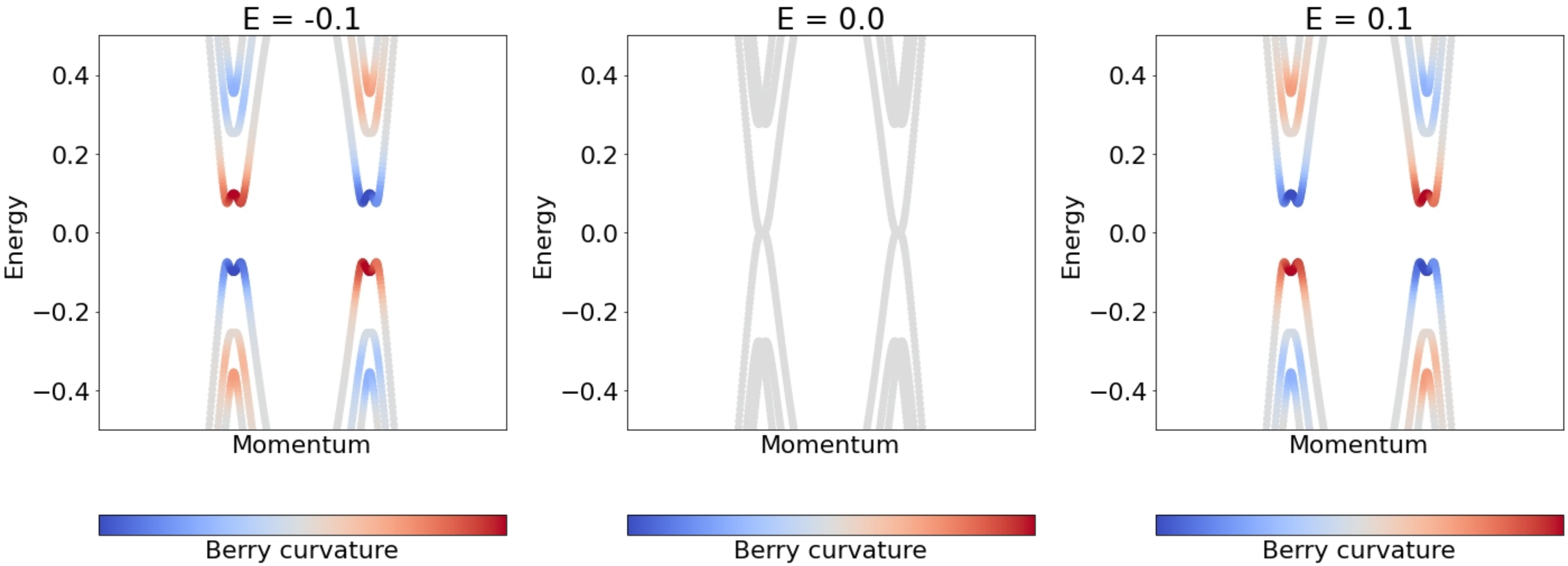
Edge states appear in the presence of a bias between layers

Biased graphene bilayers



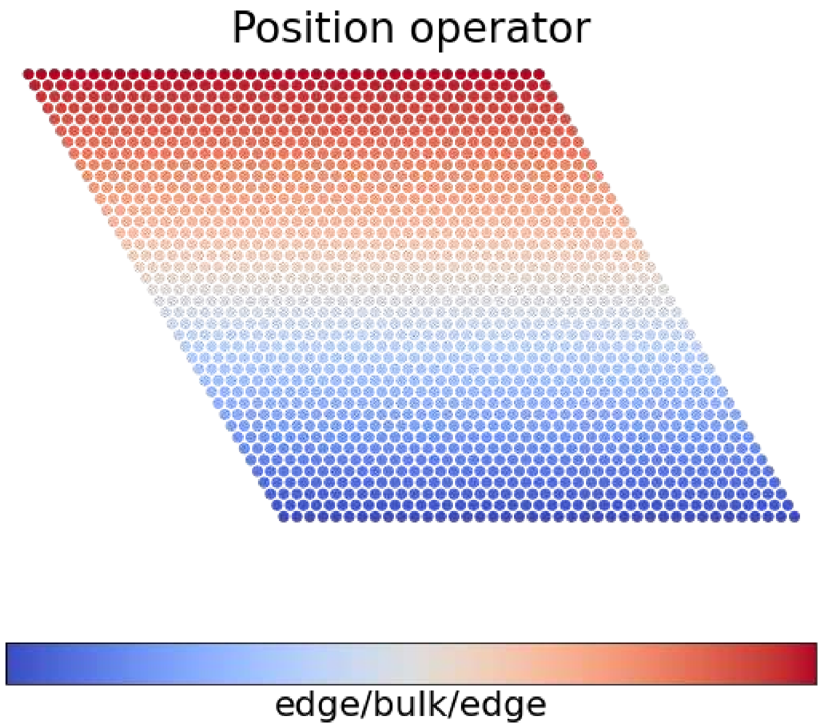
A valley Hall state generates counter propagating pseudo-helical modes

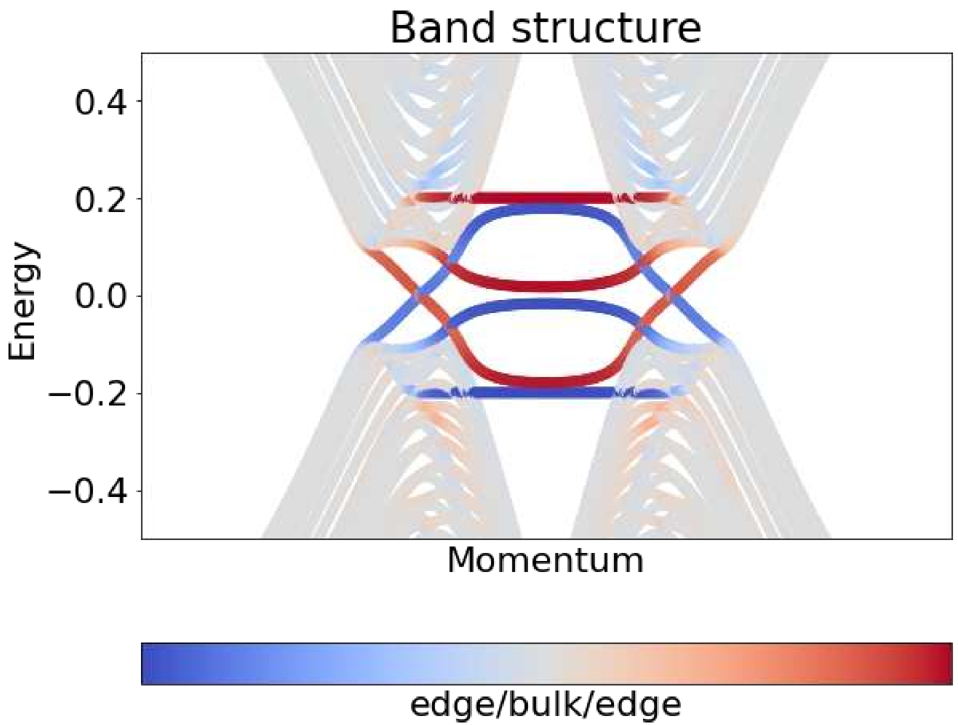
Bias controlled electronic structure in ABC trilayer graphene



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

Valley Hall states in ABC graphene multilayers





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

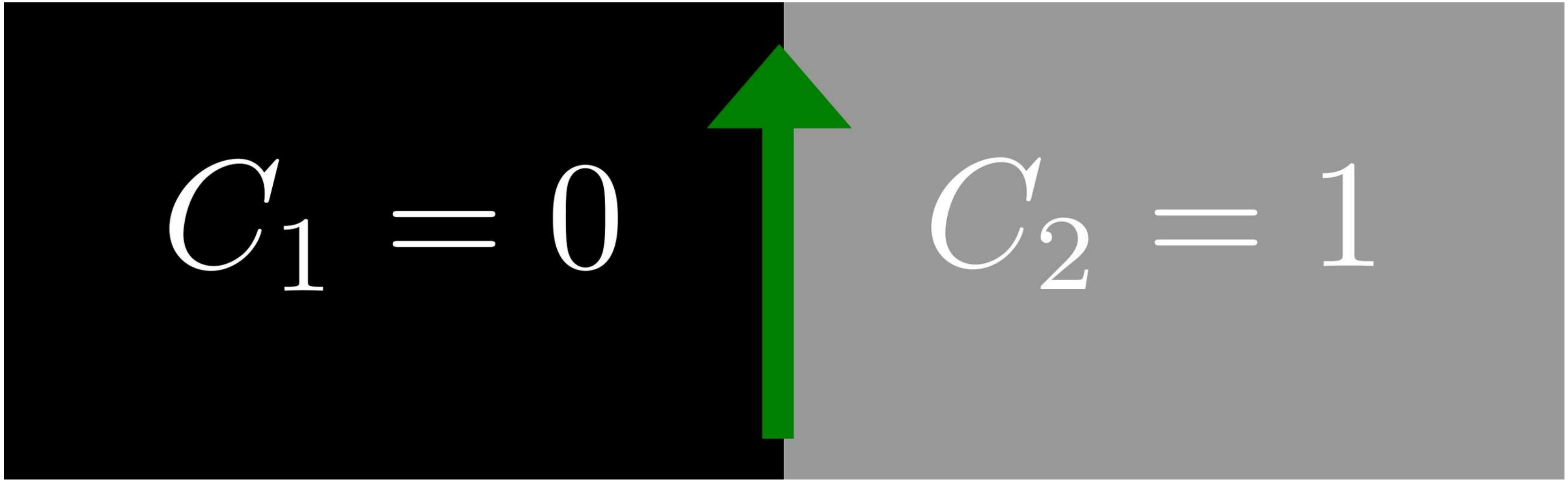
Topological phase transitions

Topological protection and edge states

Trivial system

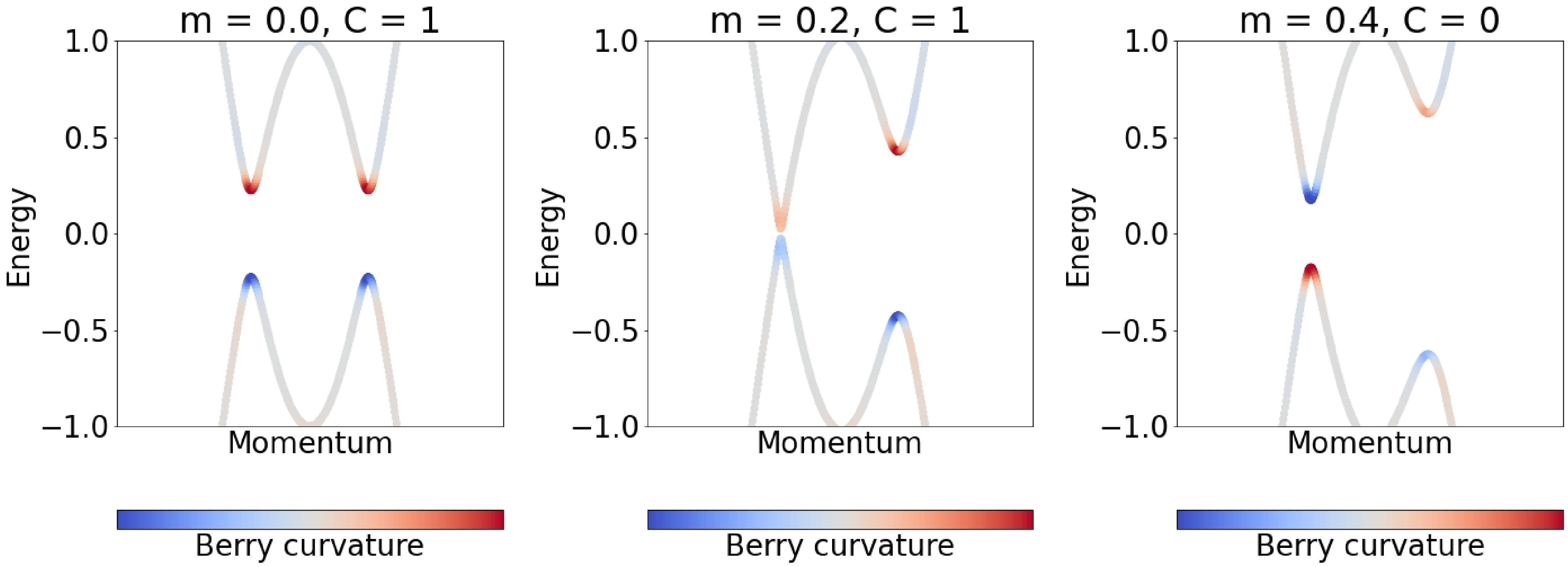
Topologically protected chiral state

Topological system



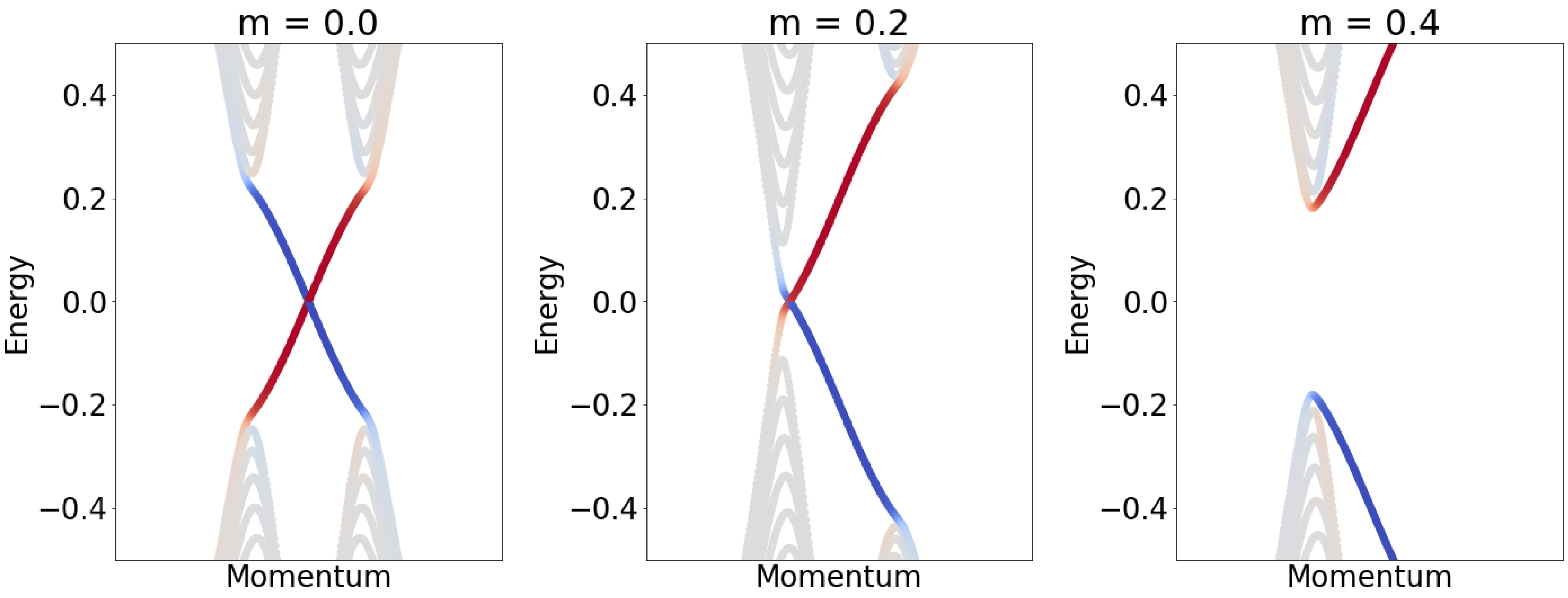
Transforming between Hamiltonians with different topological invariant closes a gap

Topological phase transition in the bulk, Chern insulator



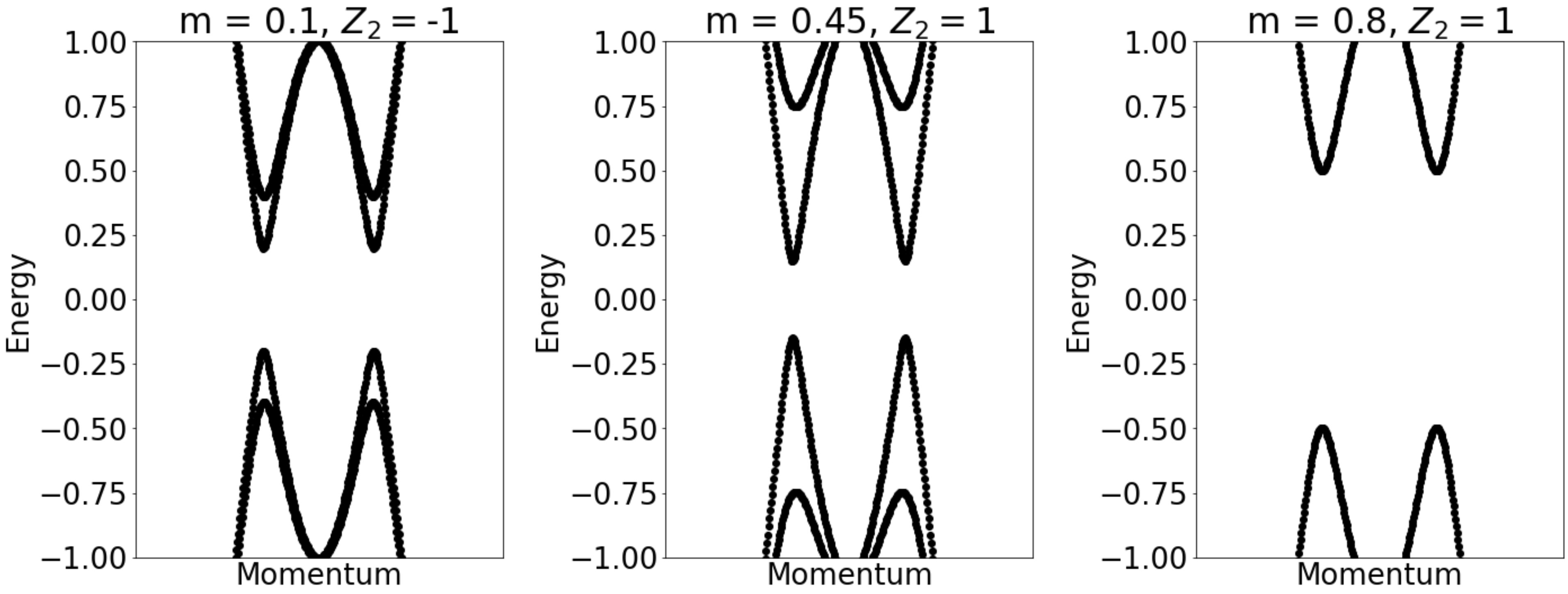
A gap closing in the bulk leads to a change in the Berry curvature of the occupied states

Topological phase transition in the edge, Chern insulator



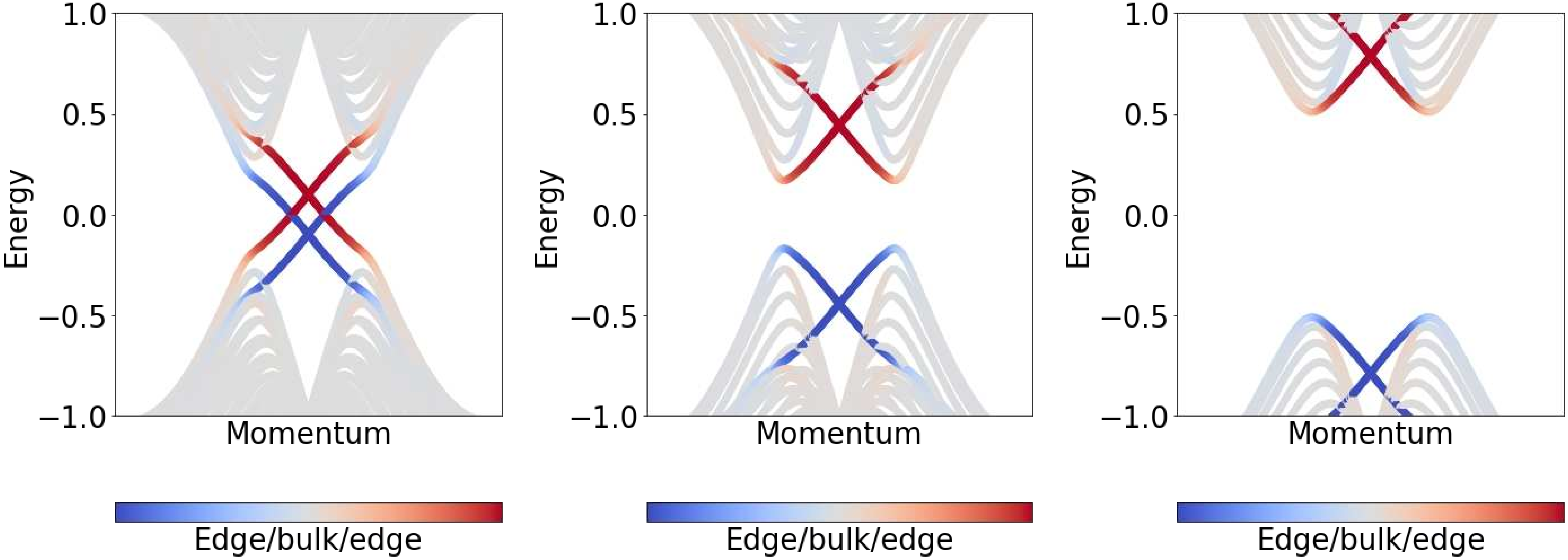
A gap closing in the bulk leads to a change in the chiral edge states

Topological phase transition in the bulk, quantum spin Hall insulator



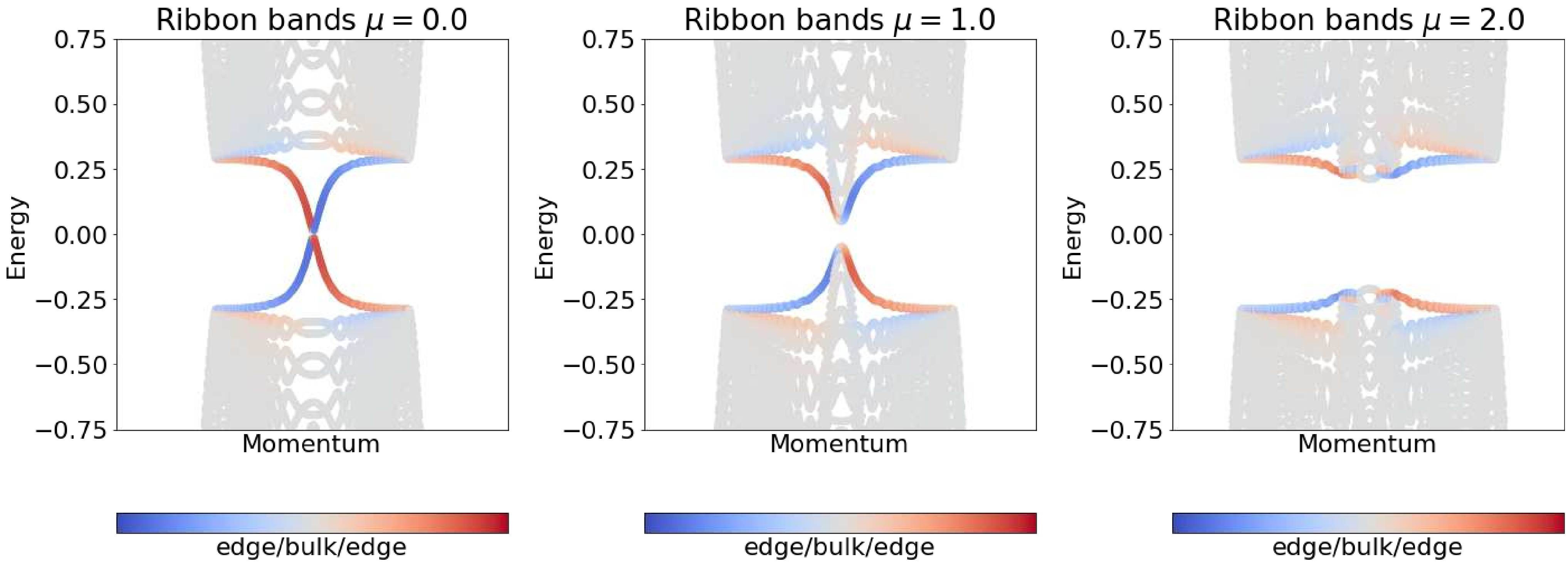
A gap closing in the bulk leads to a change in the Z_2 invariant

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

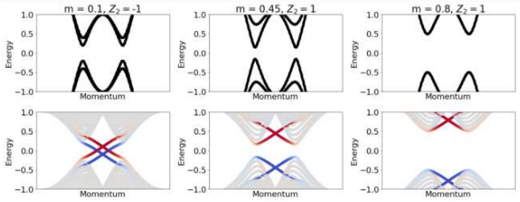
https://github.com/joselado/jyvaskyla_summer_school_2022/blob/main/sessions/session5.ipynb

The tasks during the exercise sessions

You will see examples with the code

```python
from pyqula import geometry, ribbon, topology
ms = np.linspace(0.1,0.8,3) # number of plots

ii = 1 # counter for the subplots
for m in ms:
    # bulk electronic structure and topological invariant
    plt.subplot(2,len(ms),ii) # new subplot
    g = geometry.honeycomb_lattice() # honeycomb lattice
    h = g.get_hamiltonian(tij=[1.,0.]) ; h.set_filling(0.5) # generate the Hamiltonian at half filling
    h.add_soc(0.1) # add SOC that drives QSH
    h.add_sublattice_imbalance(m) # add a sublattice imbalance
    (k,e) = h.get_bands() # compute band structure
    plt.scatter(k,e,c="black") ; plt.xlabel("Momentum") ; plt.ylabel("Energy")
    plt.xticks([]) ; plt.ylim([-1.,1.]) # plot
    z2 = topology.z2_invariant(h) # compute the Z2 invariant
    plt.title("m = "+str(np.round(m,2))+", $Z_2 =$"+str(z2)) # set the title
    # now electronic structure of a ribbon
    plt.subplot(2,len(ms),ii+len(ms)) # new subplot
    h = ribbon.bulk2ribbon(h,n=20) # create a ribbon
    (k,e,c) = h.get_bands(operator="yposition") # compute band structure
    plt.scatter(k,e,c=c) ; plt.xlabel("Momentum") ; plt.ylabel("Energy") ; plt.xticks([]) ; plt.ylim([-1.,1.])
    ii += 1
plt.tight_layout() # adjust the subplots
```



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