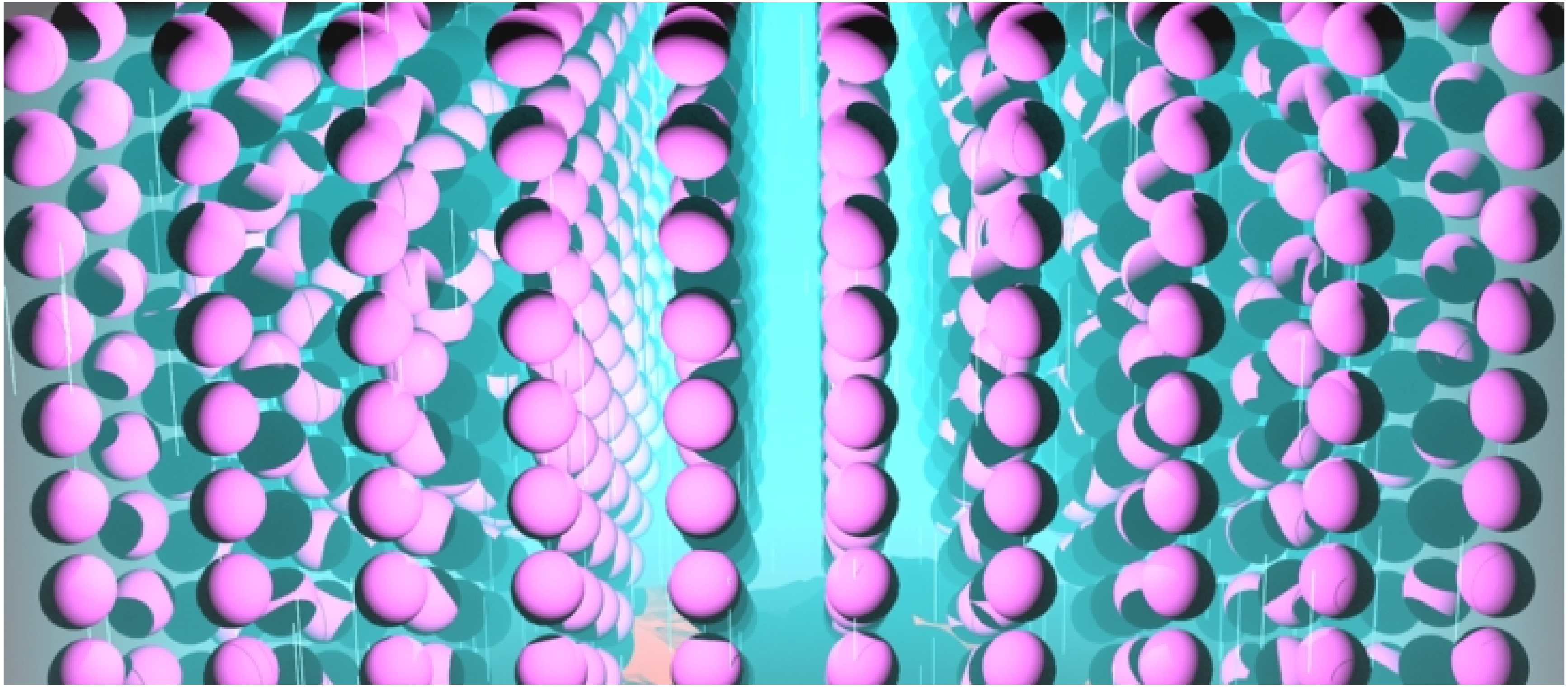
Summary



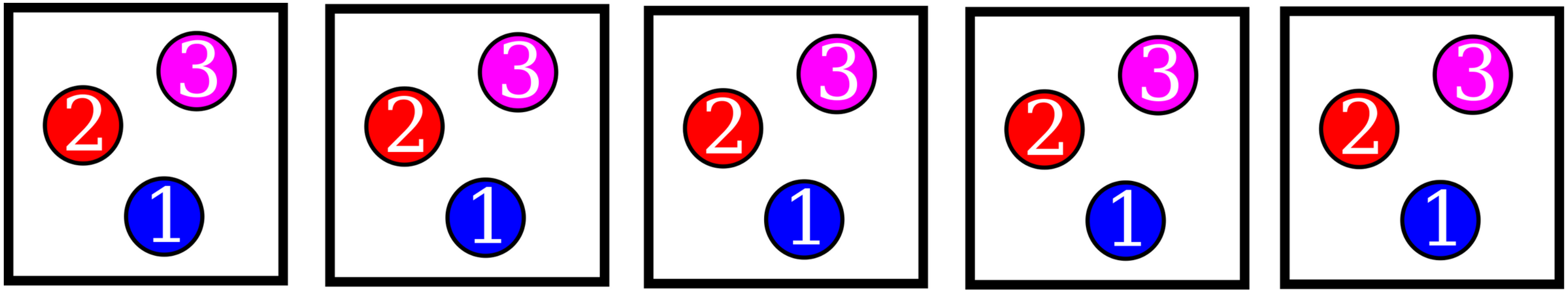
May 29th 2023

Today’s plan

- A review of band structures (and a step beyond)
- A review of superconductivity (and a step beyond)
- A review of topology (and a step beyond)

Band structure, a reminder

Multi-orbital band-structures

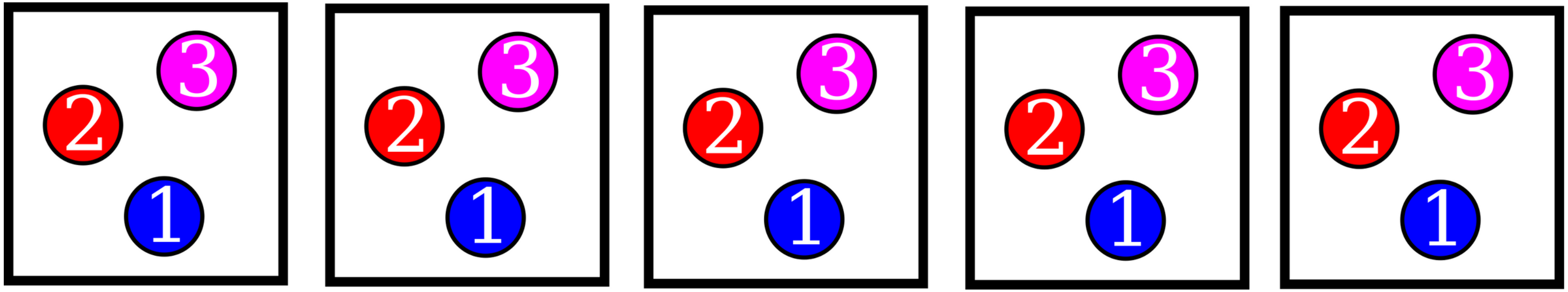


$$c^{\dagger}_{\alpha,n}$$

index of the orbital in the unit cell

Index of the unit cell

Multi-orbital band-structures



Cell #1 Cell #2 Cell #3 Cell #4 Cell #5

$$H = \sum_{n,\alpha,\beta} \underbrace{t_{\alpha\beta}}_{\text{Intra-cell hoppings}} c^\dagger_{\alpha,n} c_{\beta,n} + \sum_{n,\alpha,\beta} \underbrace{\gamma_{\alpha\beta}}_{\text{Inter-cell hoppings}} c^\dagger_{\alpha,n} c_{\beta,n+1} + h.c.$$

Multi-orbital band-structures

$$H = \sum_{n,\alpha,\beta} t_{\alpha\beta} c^\dagger_{\alpha,n} c_{\beta,n} + \sum_{n,\alpha,\beta} \gamma_{\alpha\beta} c^\dagger_{\alpha,n} c_{\beta,n+1} + h.c.$$

Unitary transformation

$$\Psi^\dagger_{\phi,\alpha} \sim \sum_{n,\beta} e^{i\phi n} U_{\alpha\beta} c^\dagger_{n,\beta} \qquad H = \sum_{\phi,\alpha} \epsilon_{\phi,\alpha} \Psi^\dagger_{\phi,\alpha} \Psi_{\phi,\alpha}$$

$\epsilon_{\phi,\alpha}$ **are the eigenvalues of the matrix**

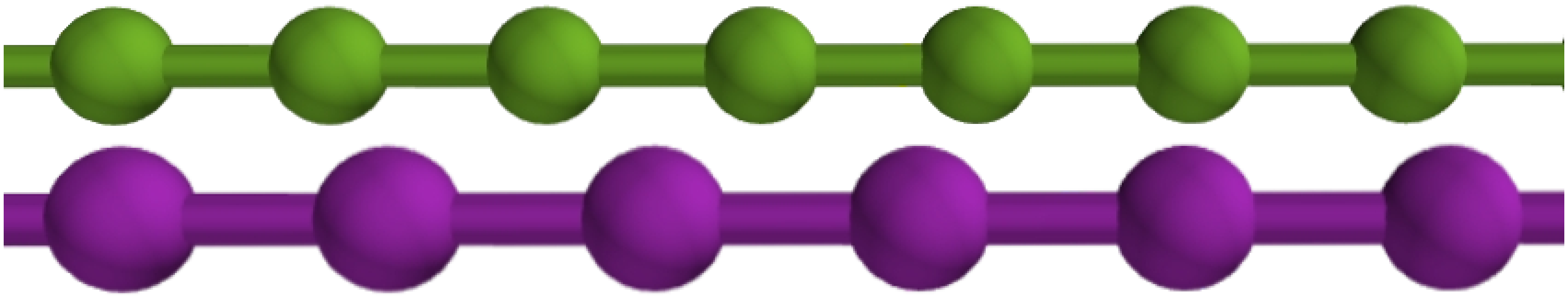
$$h(\phi) = t_{\mu\nu} + \gamma_{\mu\nu} e^{i\phi} + h.c.$$

But what if we do not have periodicity in the system?

Superpotentials and quasiperiodicity

A minimal moire potential

Let us now take a one dimensional superlattice



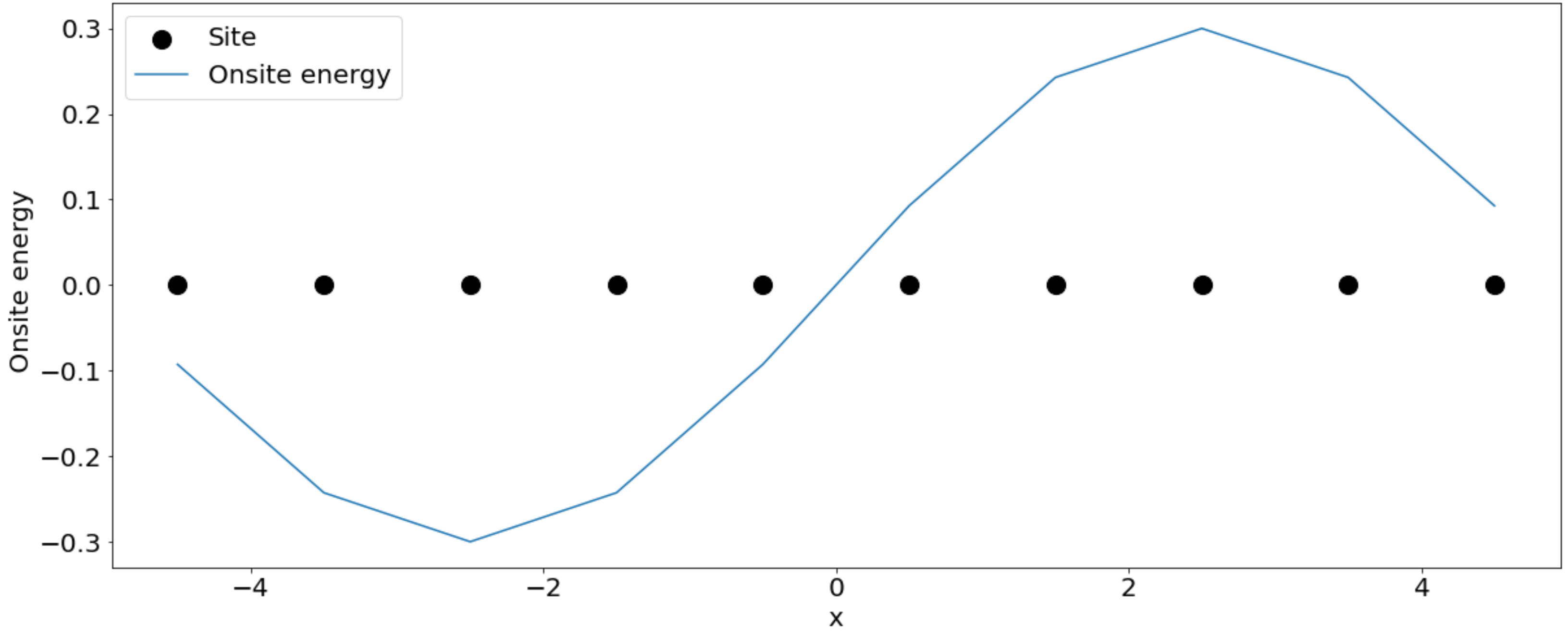
We have now two length scales

The lattice constant of the top system
The lattice constant of the bottom

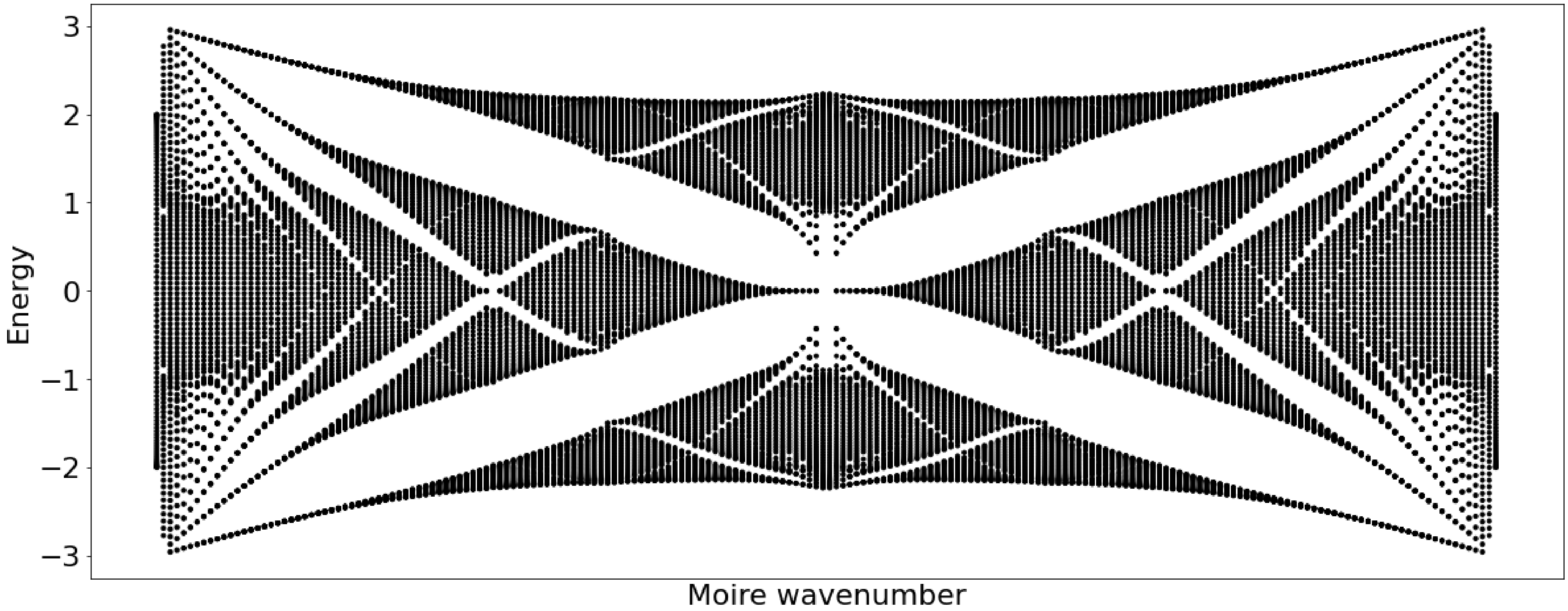
Let us see how the electronic structure gets modified by the superlattice effect

A minimal moire potential

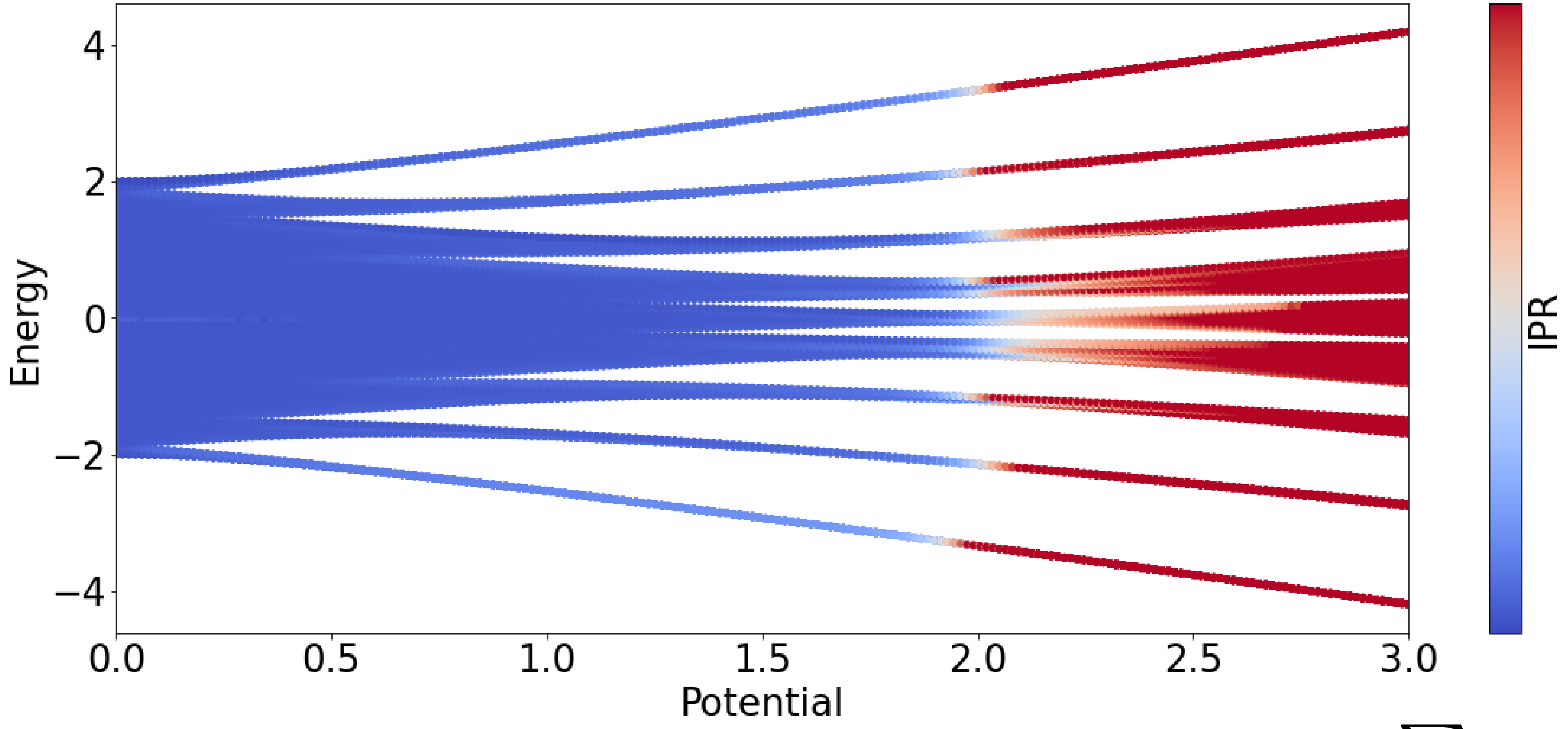
$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + \lambda \sum_n \cos(qn) c_n^\dagger c_n$$



Spectrum as a function of the moire wavevector



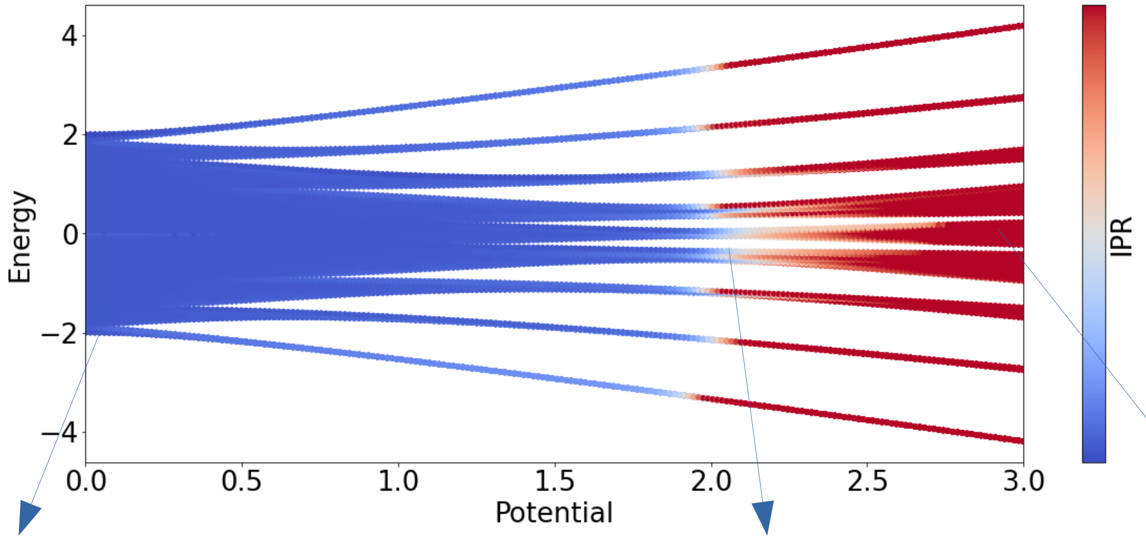
Superpotentials and criticality



$$IPR = \sum_r |\Psi(r)|^4$$

Moire potentials can give rise to critical wavefunctions

Superpotentials and criticality



$$IPR = \sum_r |\Psi(r)|^4$$

Extended states

$$|\Psi(\mathbf{r})| = 1/N$$

Critical states

$$|\Psi(\mathbf{r})| = |r|^{-\alpha}$$

Localized states

$$|\Psi(\mathbf{r})| = e^{-\lambda|r|}$$

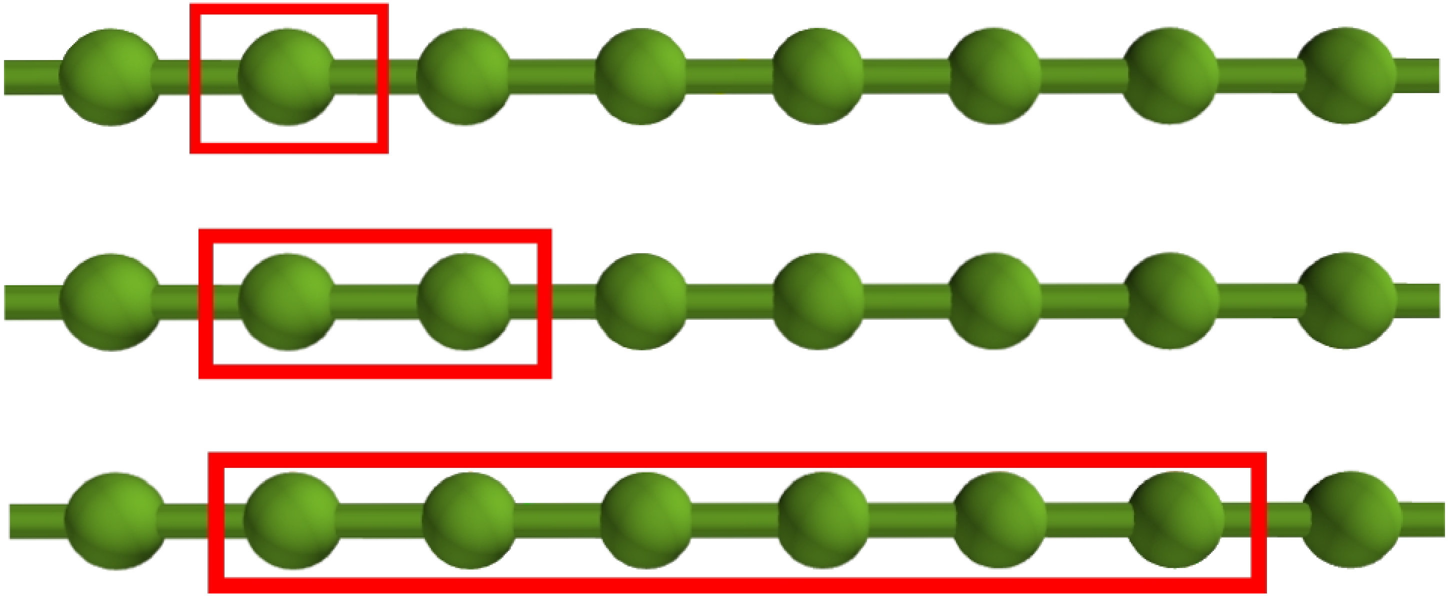
Minibands and band structure unfolding

Supercells and band folding

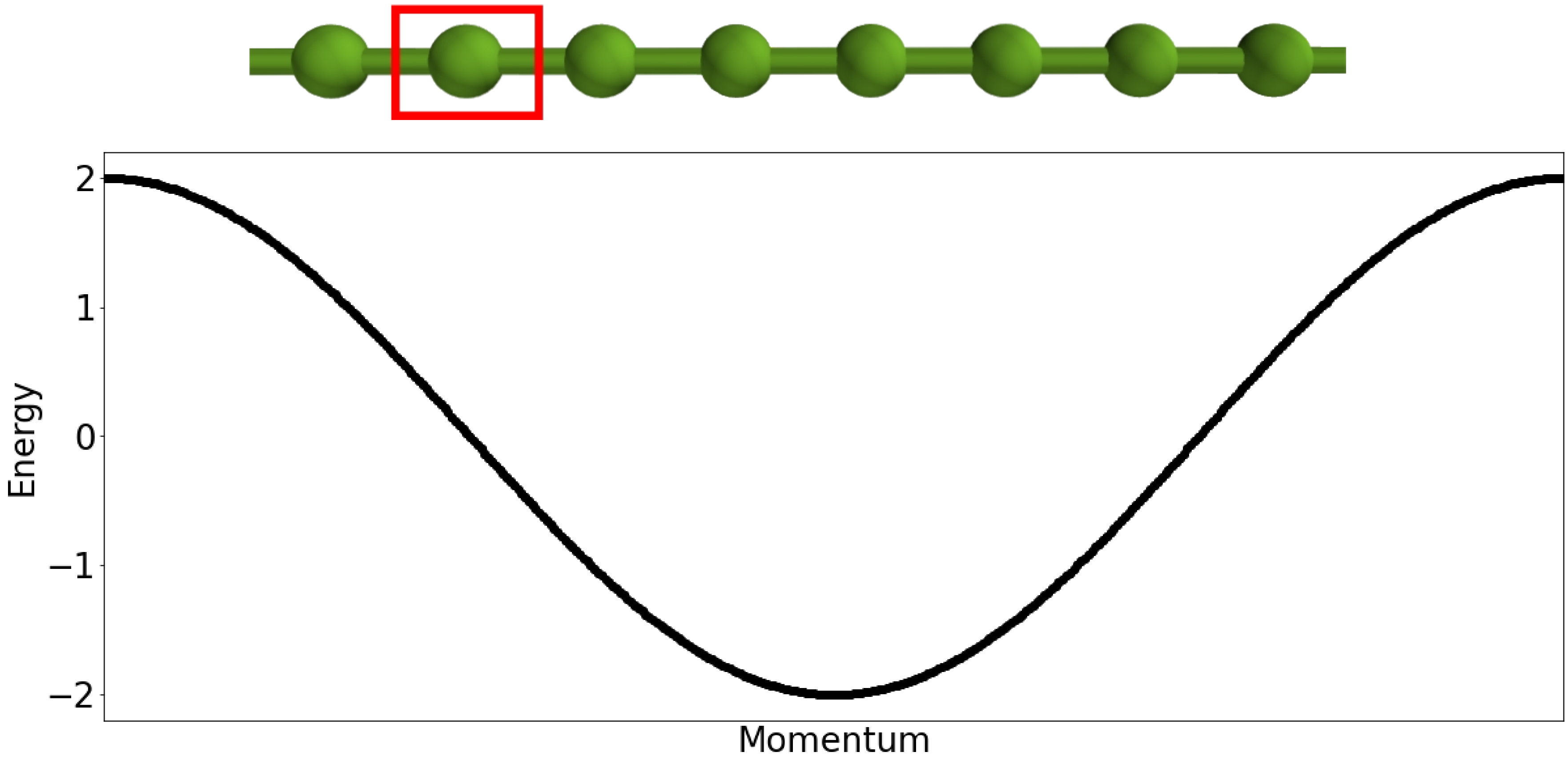
Let us take a 1D chain

$$H = \sum_n c_n^\dagger c_{n+1} + h.c.$$

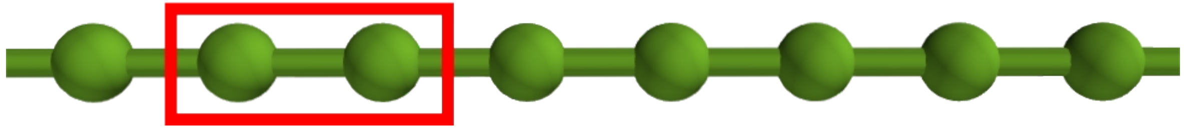
Let us see how the electronic structure changes with the unit cell

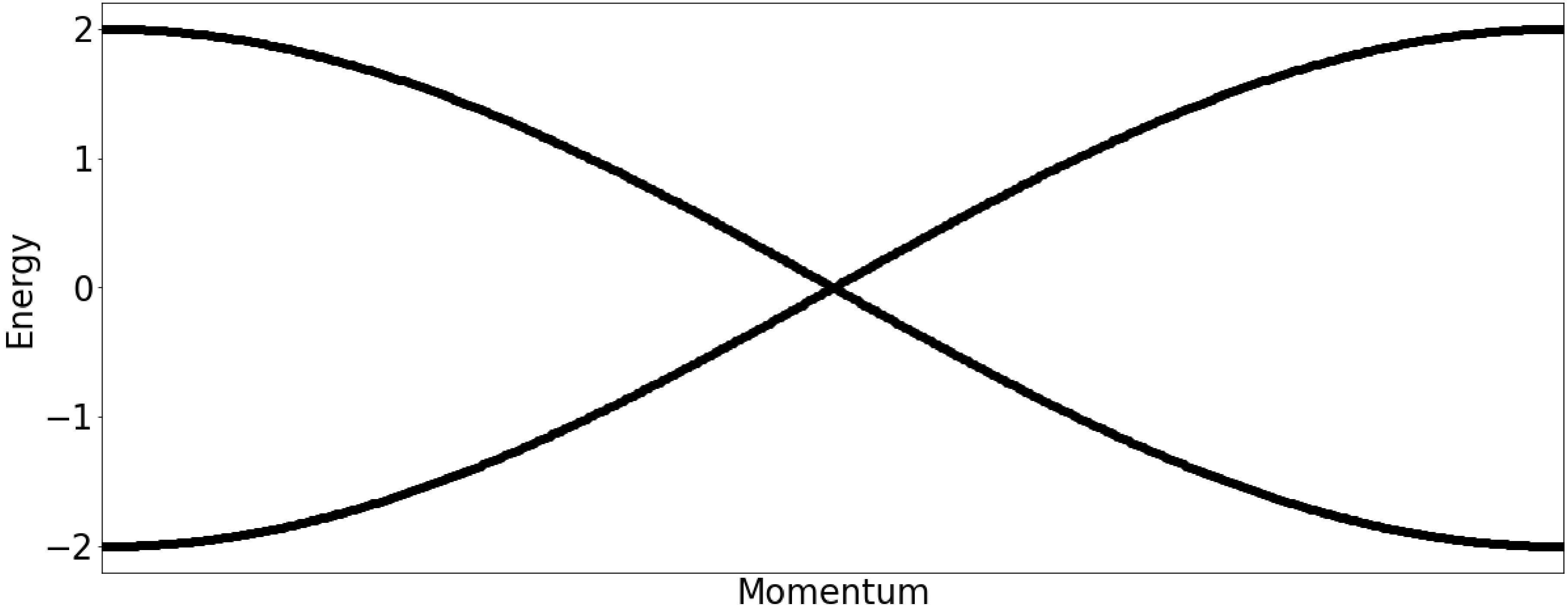


Supercells and band folding

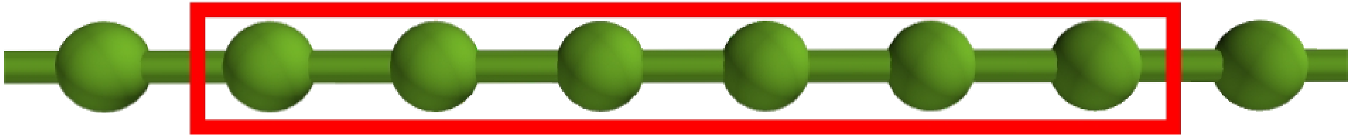


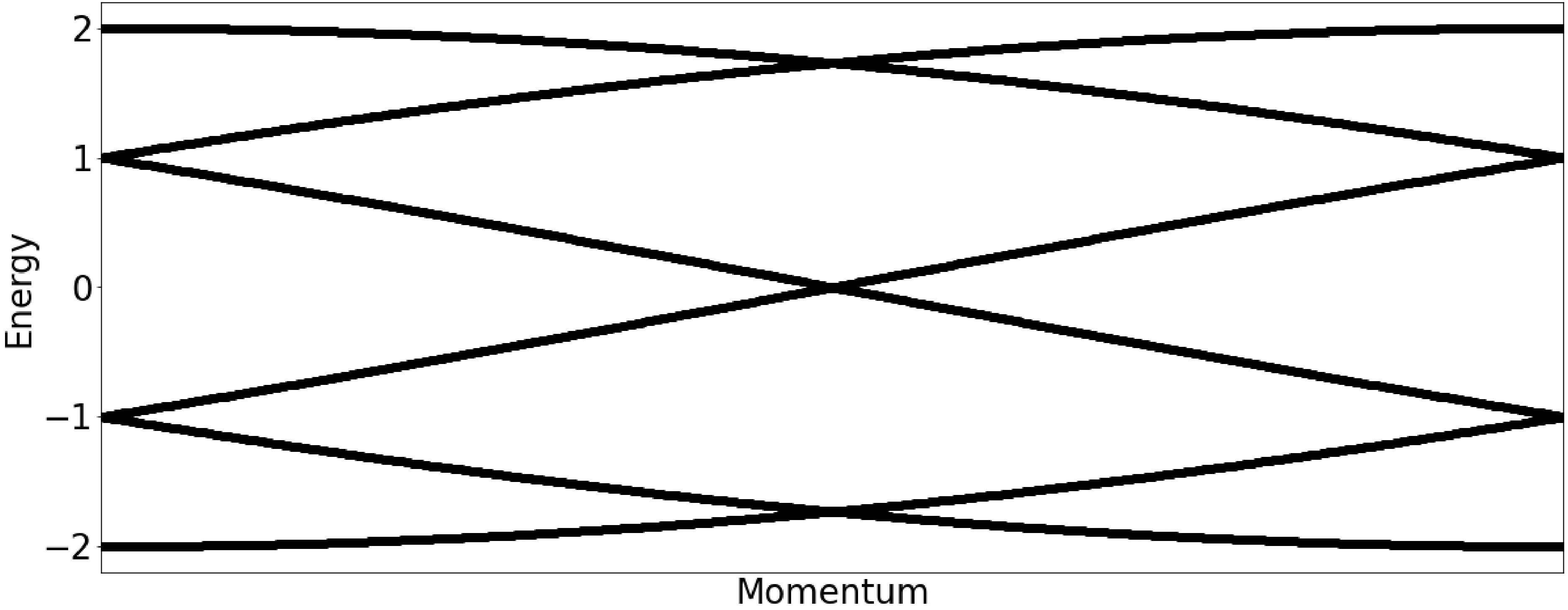
Supercells and band folding



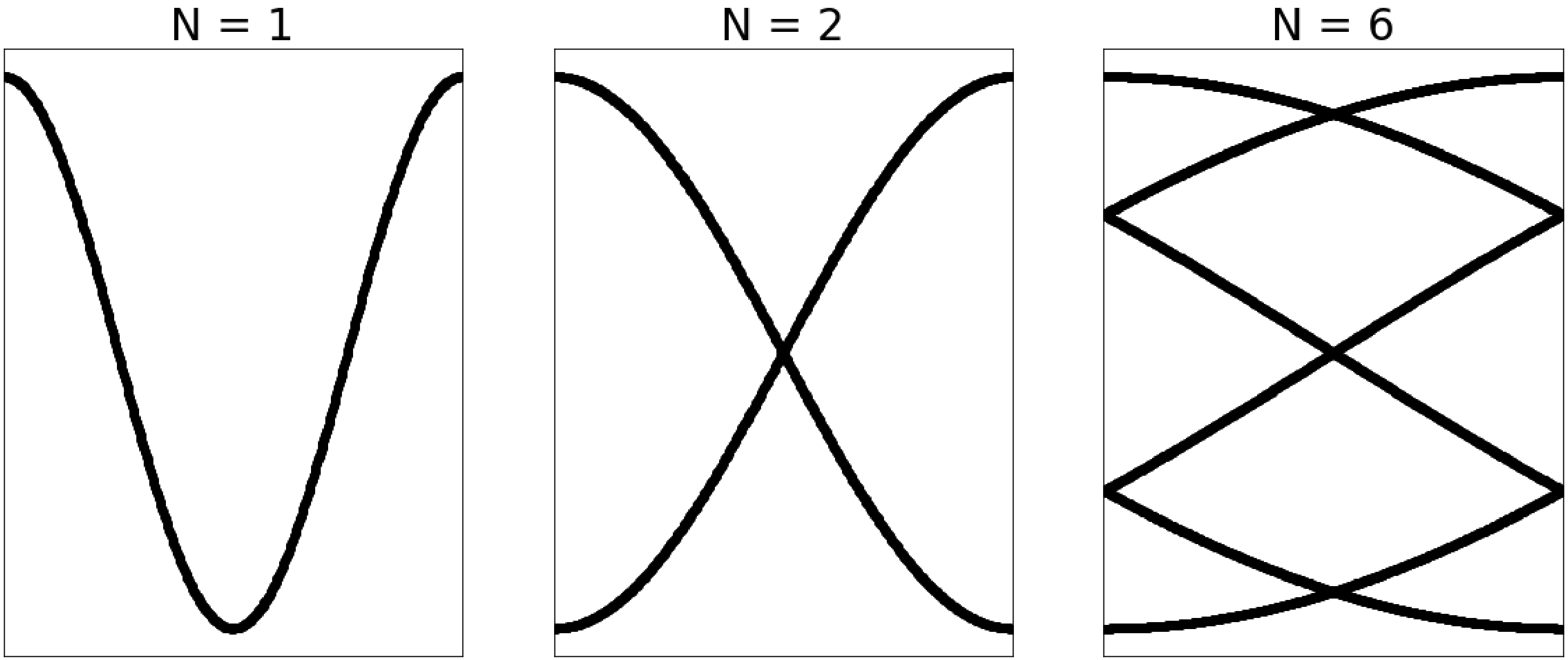


Supercells and band folding



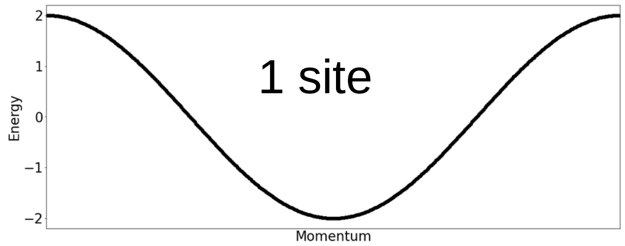


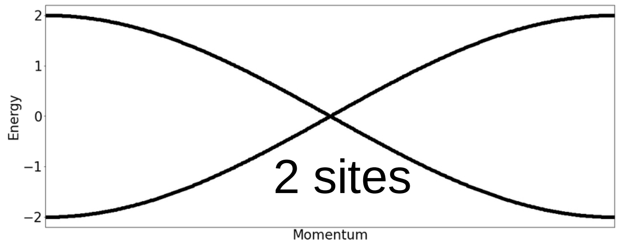
Supercells and band folding

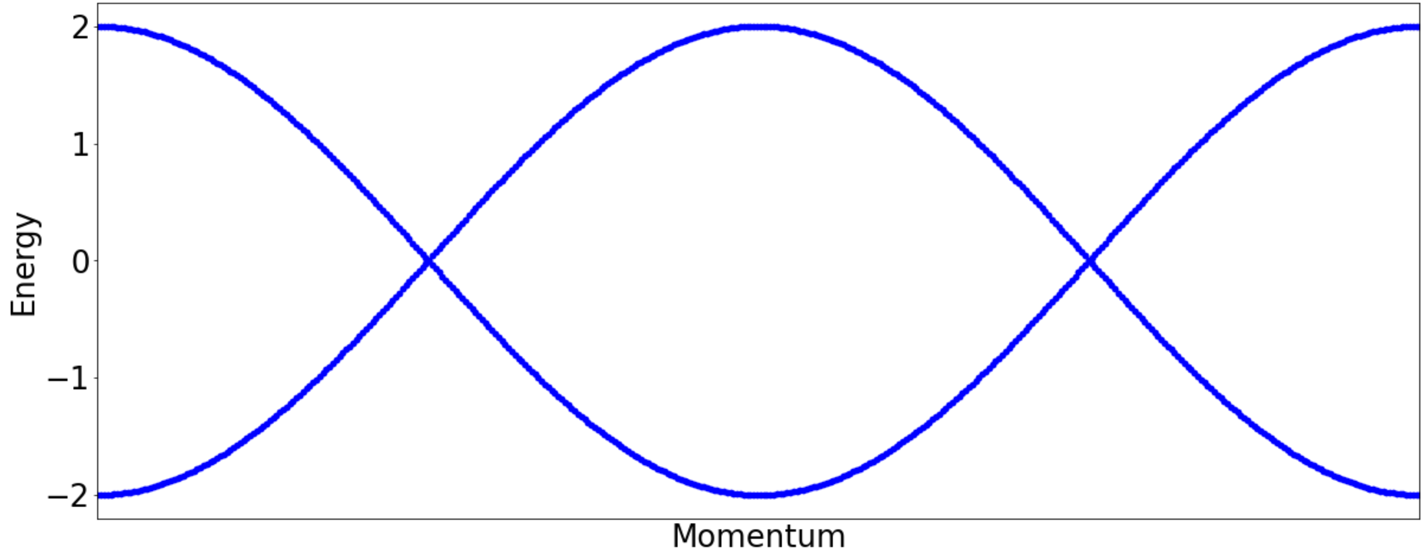


All these electronic structures represent the same physical system, but how do we see that?

Supercells and band folding

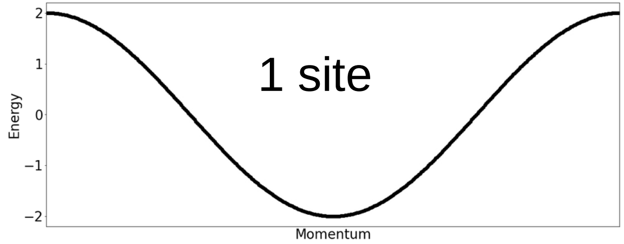


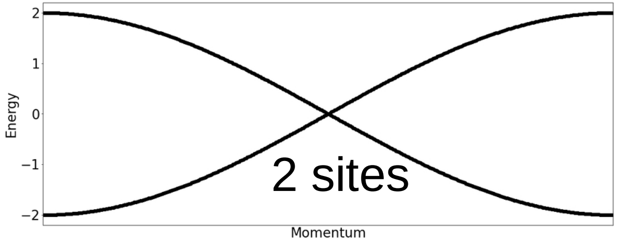


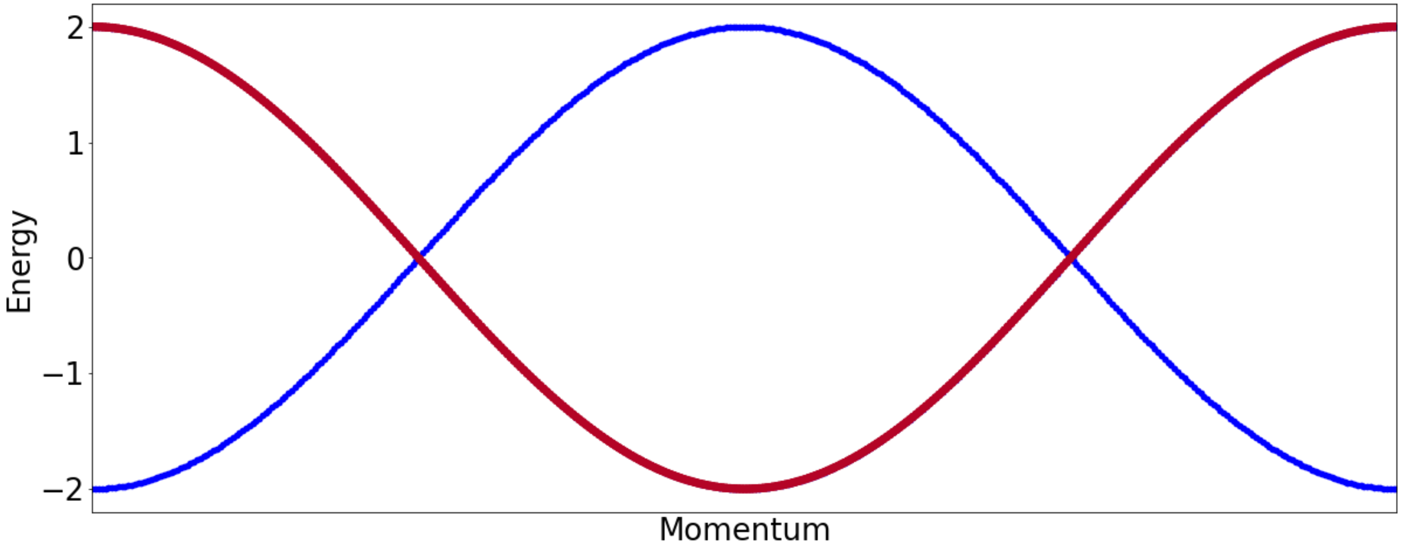


Repeating the electronic structure recovers the original electronic dispersion

Supercells and band folding

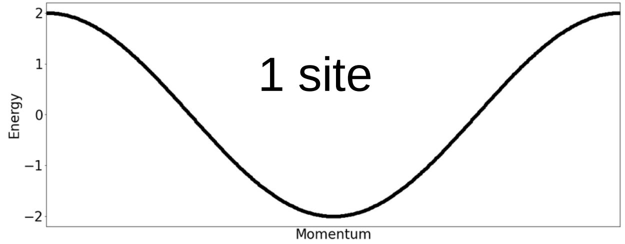


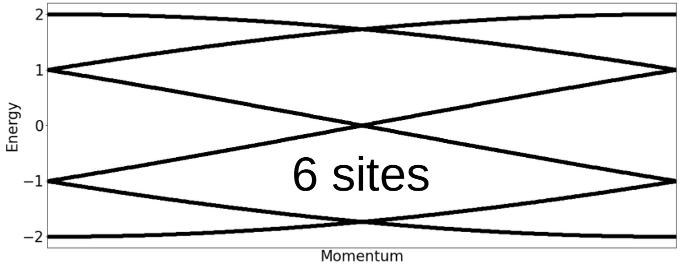


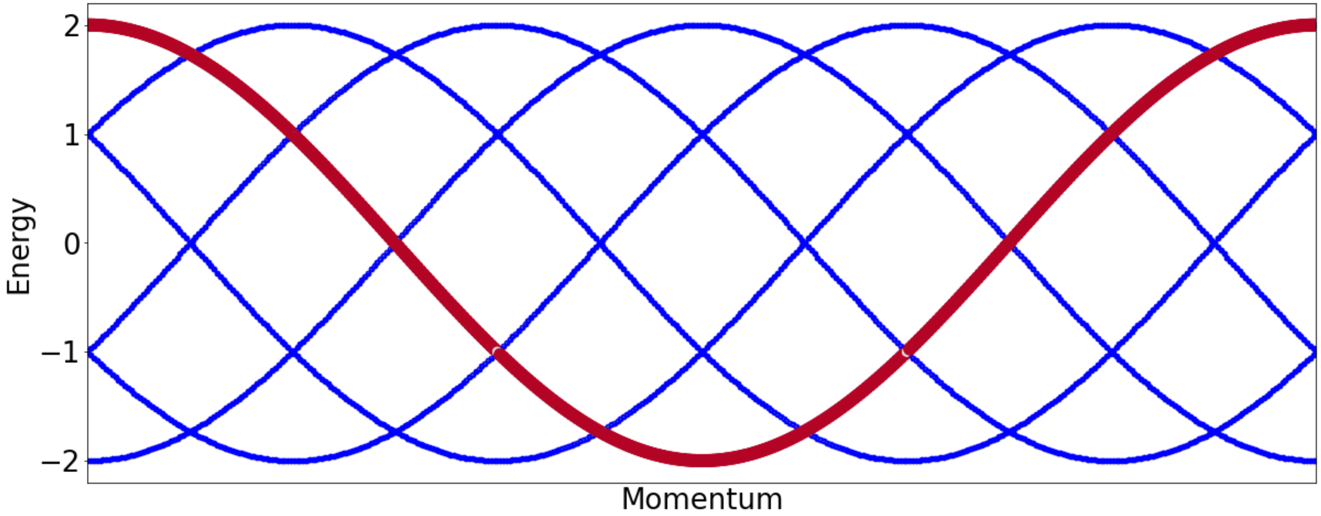


Repeating the electronic structure recovers the original electronic dispersion

Supercells and band folding



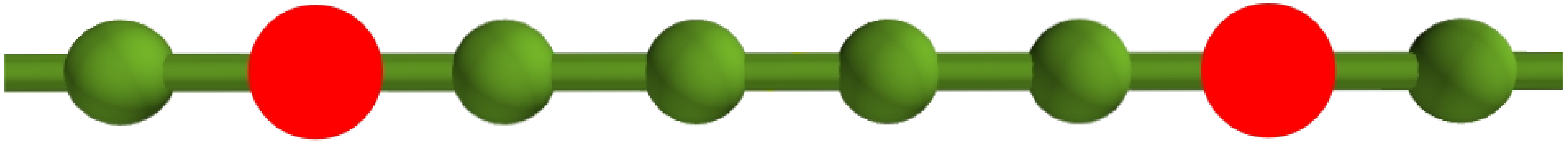




Repeating the electronic structure recovers the original electronic dispersion

Unfolding and anticrossings in superlattices

Let us now put an impurity every 6 sites (once in a supercell 6)

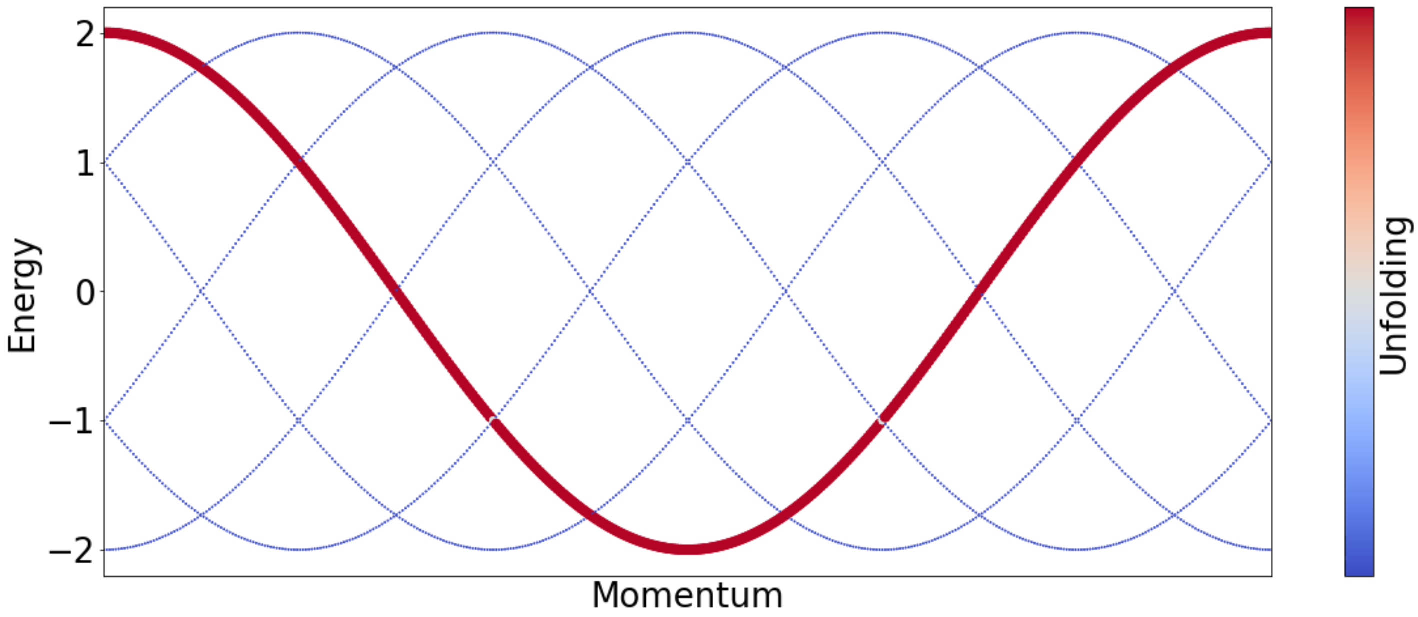


$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V_0 \sum_\alpha c_n^\dagger c_n \qquad \alpha \equiv 0 \pmod 6$$

Unfolding and anticrossings in superlattices

$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V_0 \sum_\alpha c_n^\dagger c_n$$

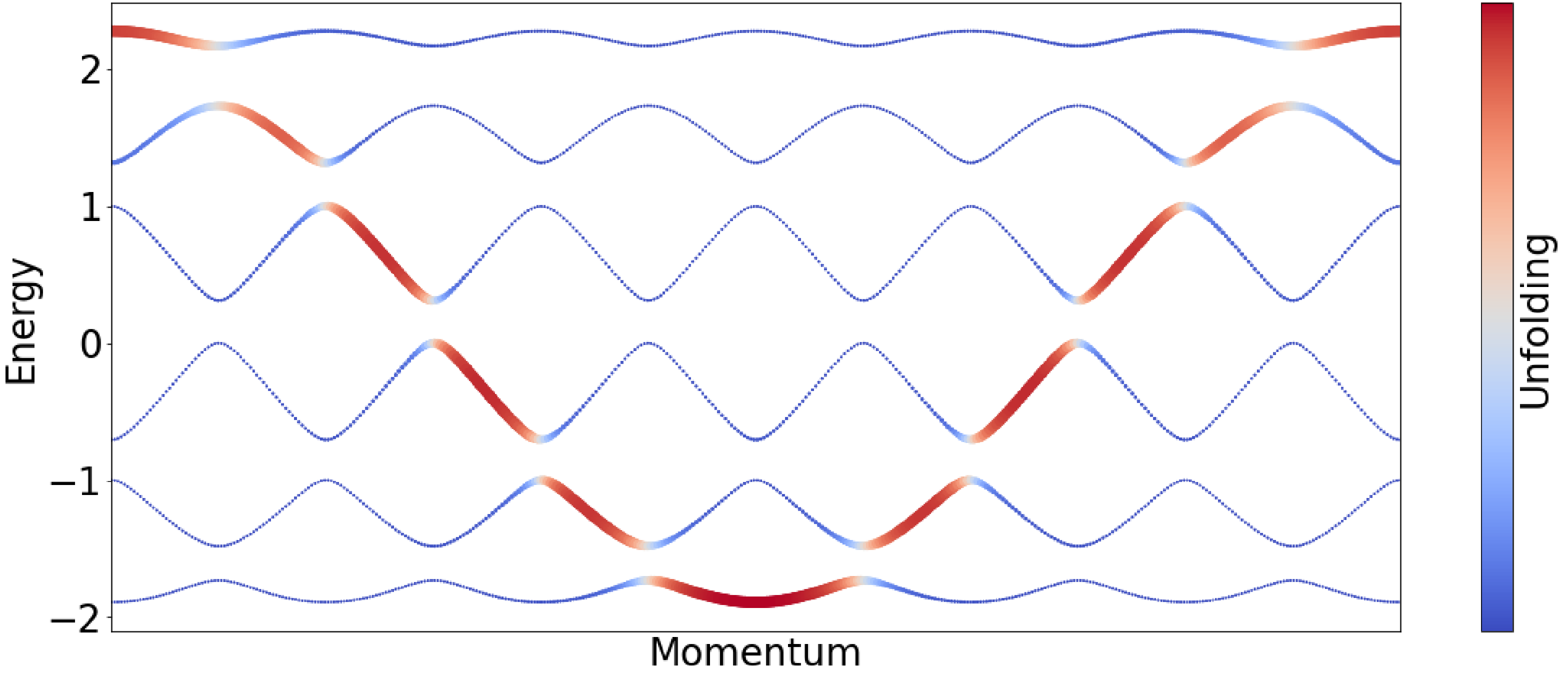
$$V_0 = 0$$



Electronic structure unfolding

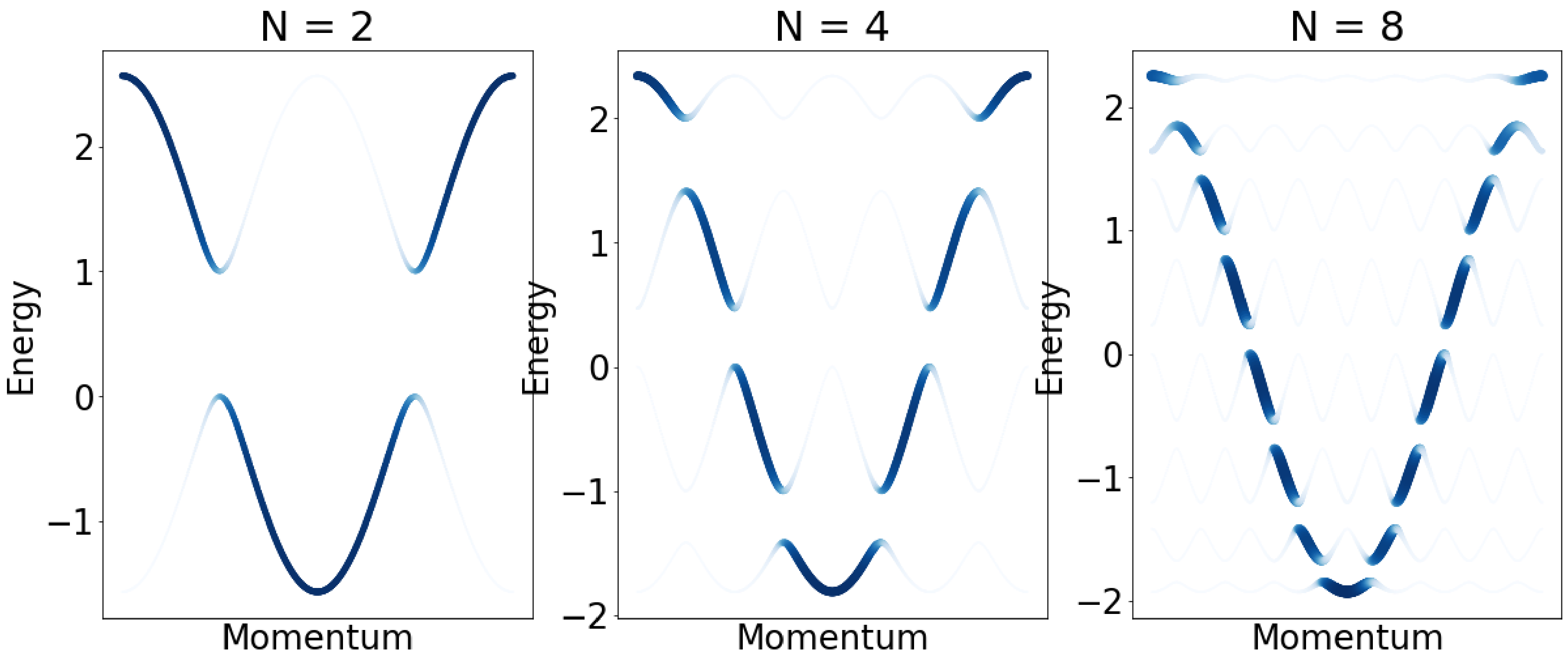
$$H = \sum_n c_n^\dagger c_{n+1} + h.c. + V_0 \sum_\alpha c_n^\dagger c_n$$

$$V_0 \neq 0$$



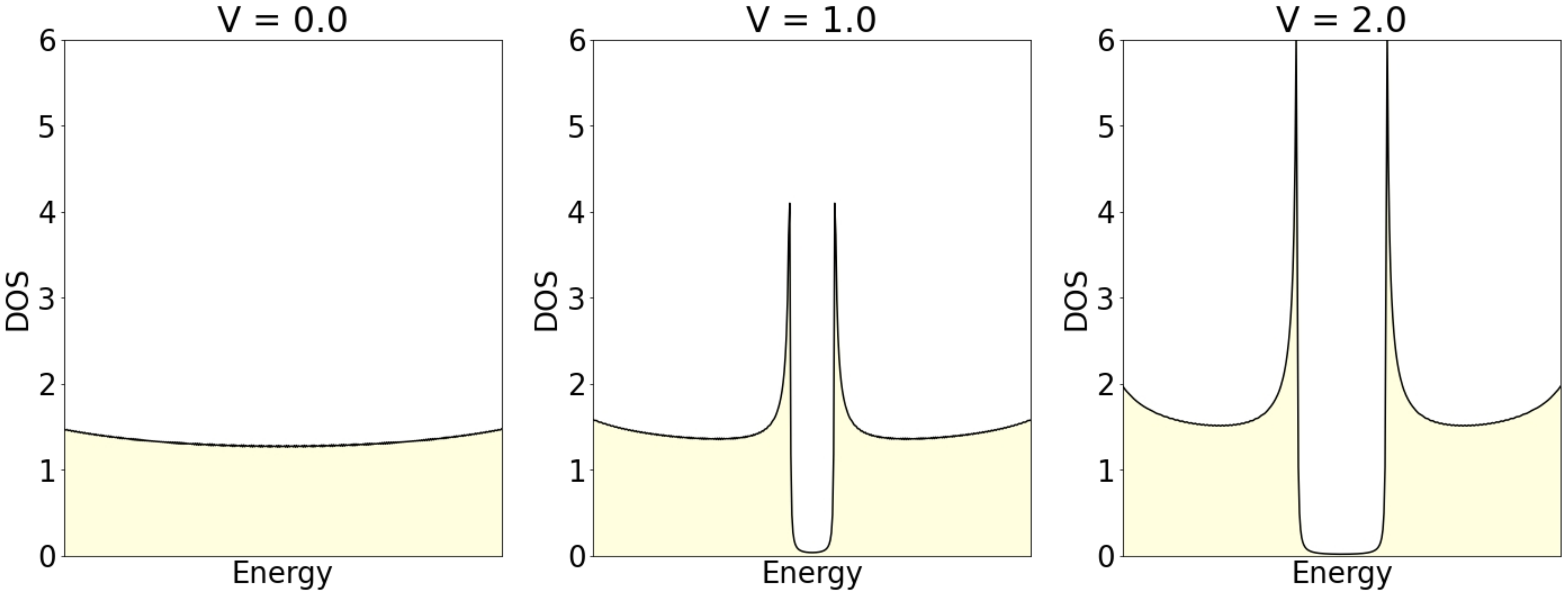
Anticrossing between the bands appear due to the superlattice potential

Electronic structure unfolding



As the periodicity of the superlattice is increased, more minibands appear

Moire electronic structure



As the strength of the miore potential increases, the density of states gets enhanced

A short exercise

To discuss

$$H = \lambda \sum_n \cos(qn) c_n^\dagger c_n$$

For a lattice with L sites, what is the value of q that makes the potential commensurate?

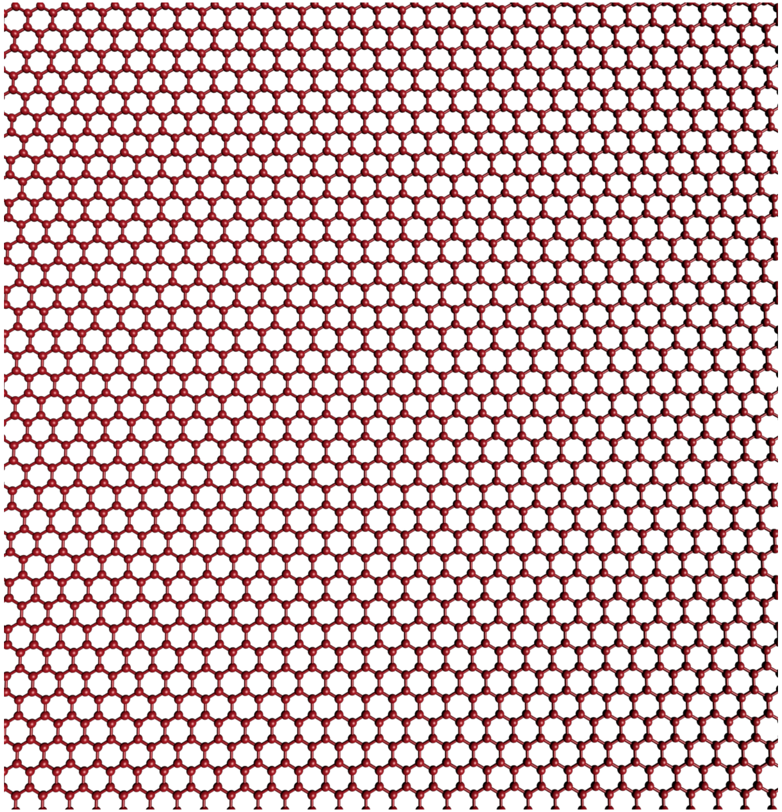
$$q = \frac{\alpha 2\pi}{L} \qquad\qquad q = \frac{\alpha \pi}{L}$$

$$\alpha = 1, 2, 3, 4, ...$$

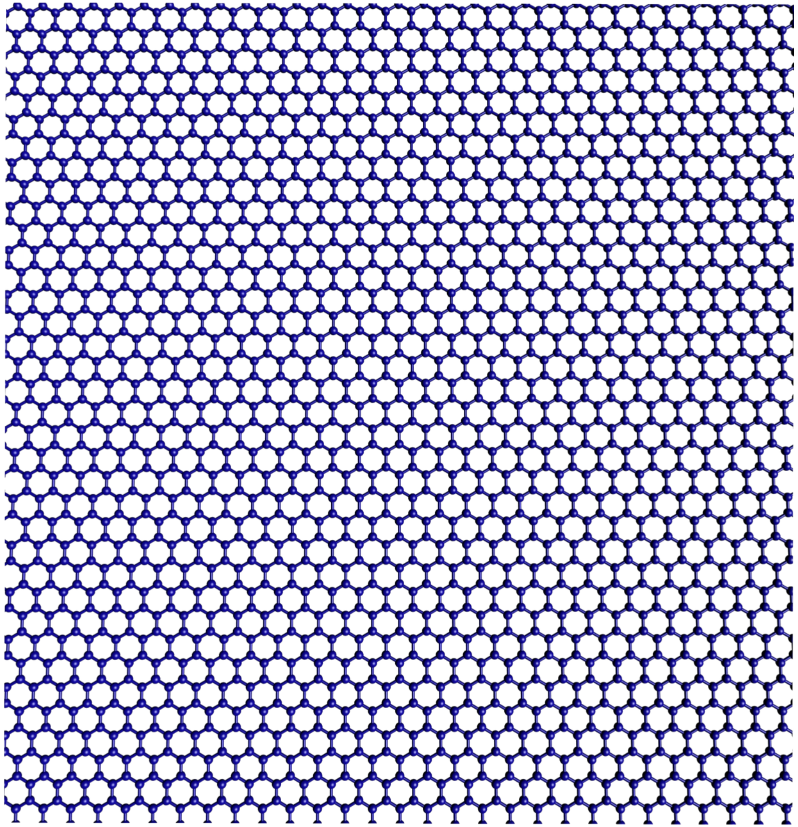
A platform for band structure folding

A bilayer van der Waals heterostructure

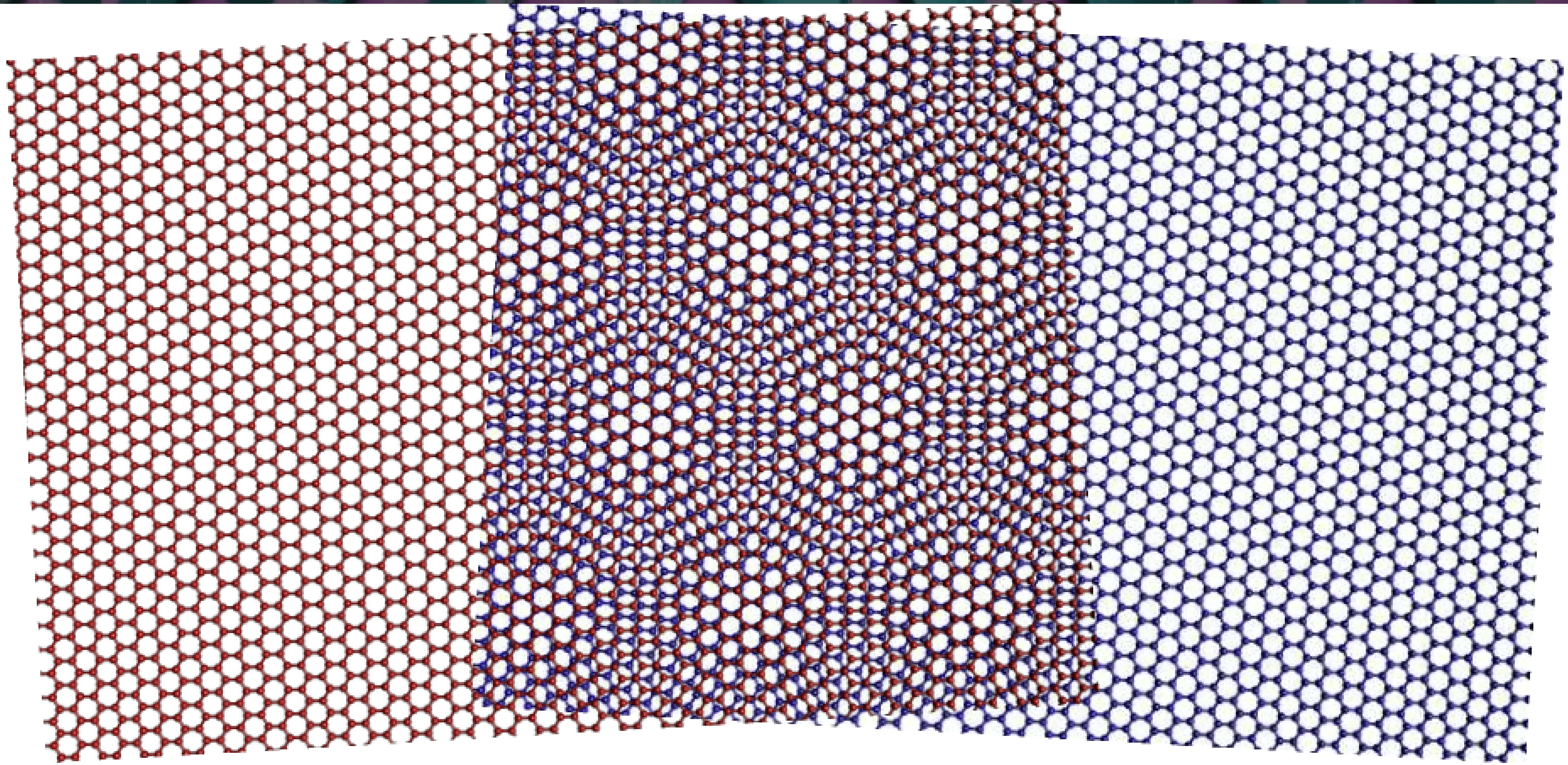
Upper graphene layer



Lower graphene layer

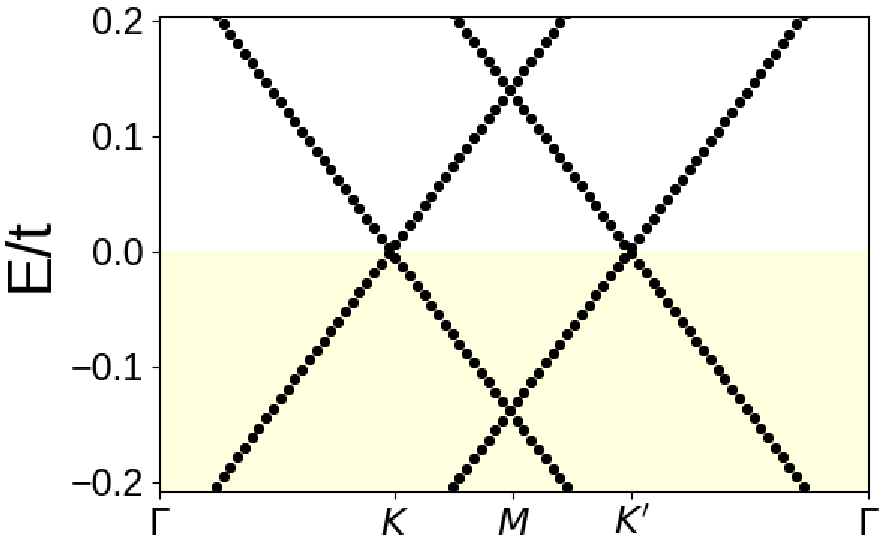


A bilayer van der Waals heterostructure

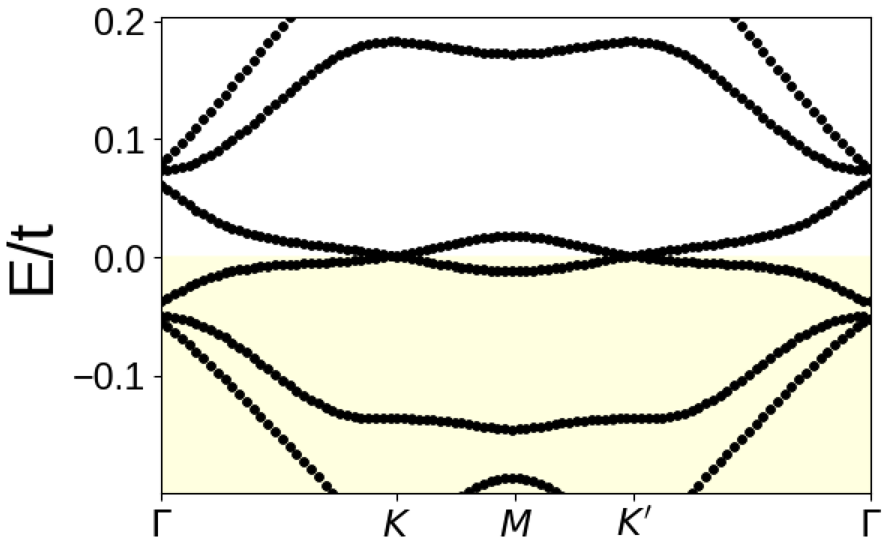


Band structure of twisted bilayer graphene

Decoupled



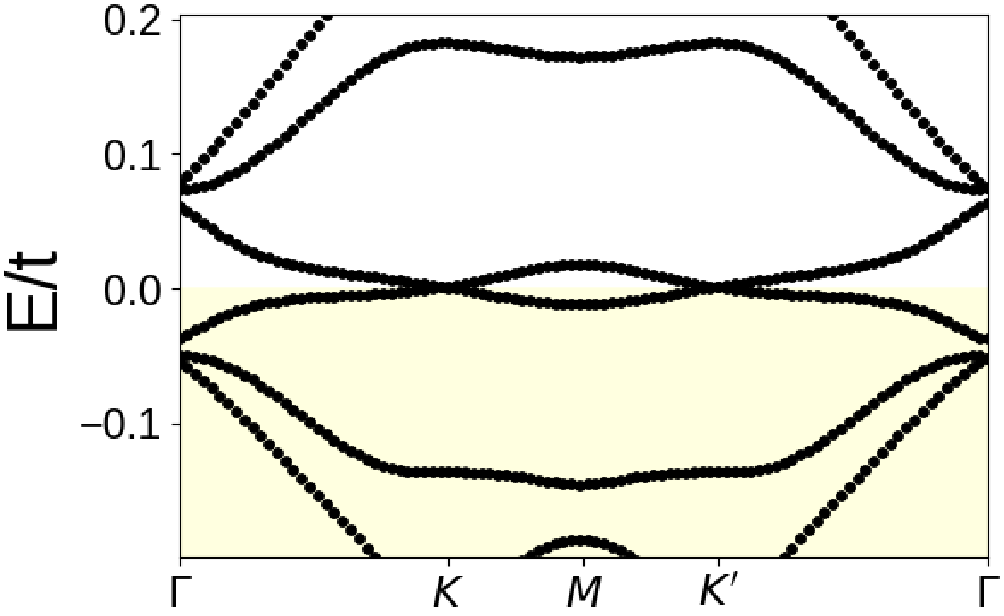
$\alpha = 1.5^\circ$



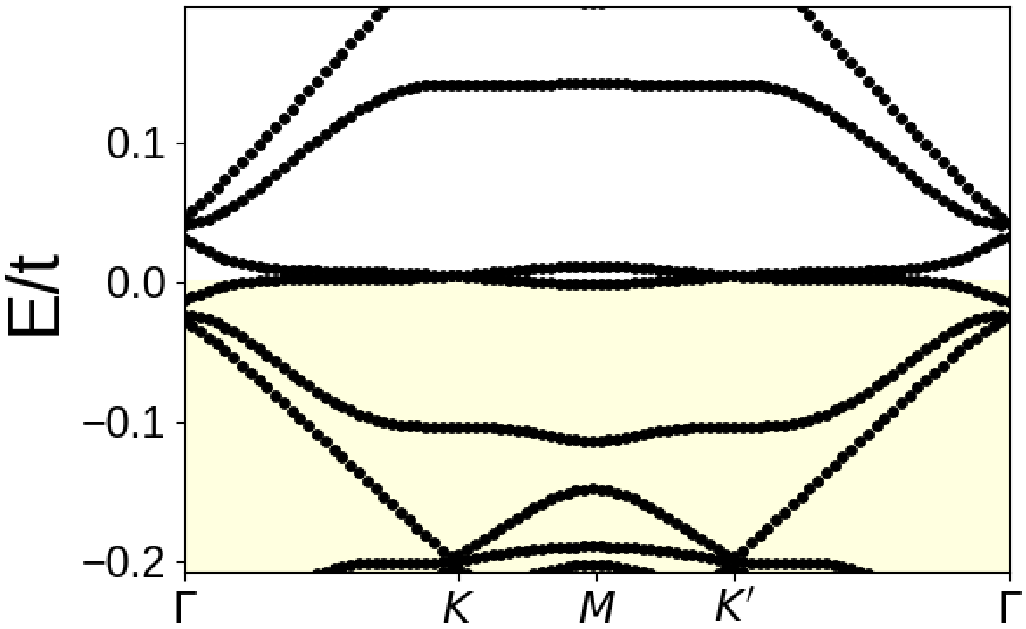
As the angle between layers in decreased, the bands become flatter

Band structure of twisted bilayer graphene

$\alpha = 1.5^\circ$

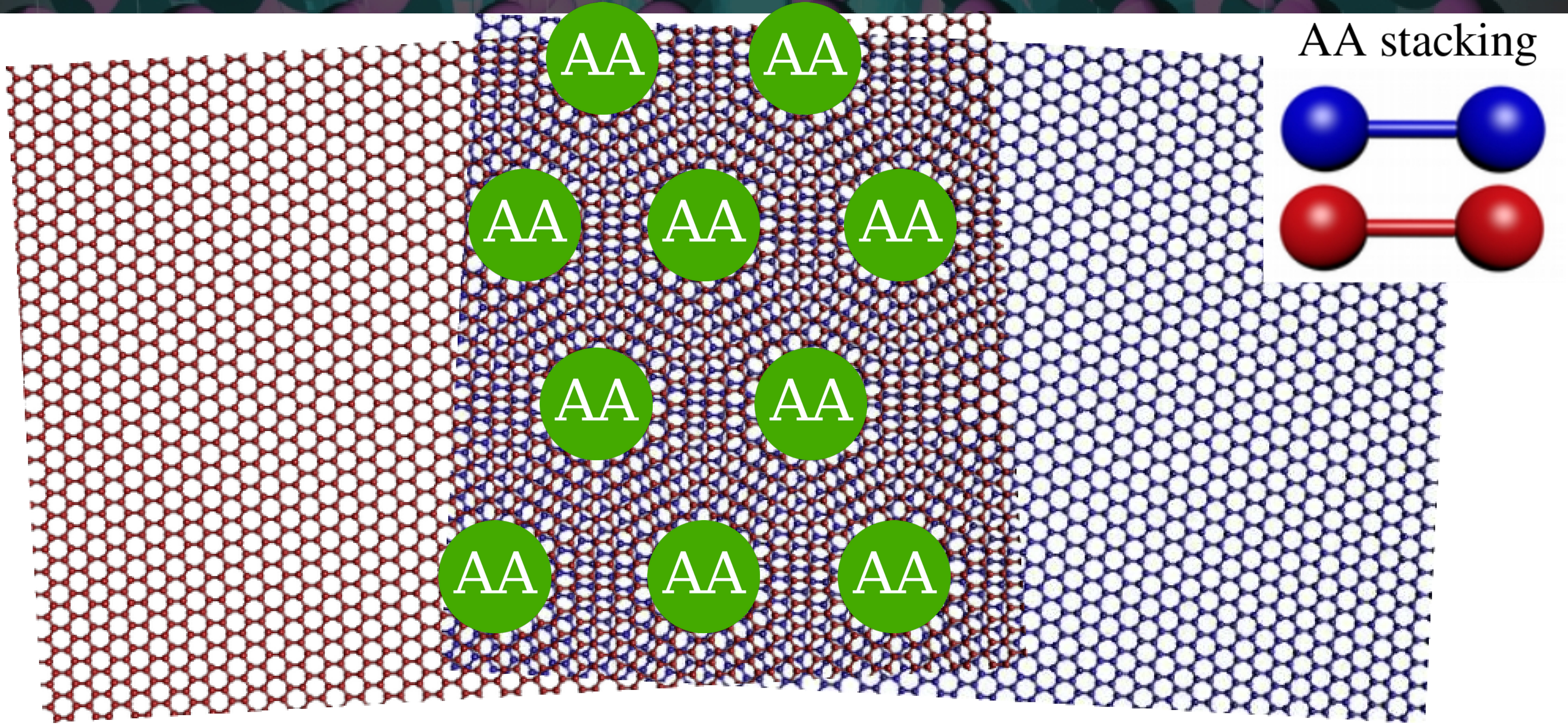


$\alpha = 1.2^\circ$

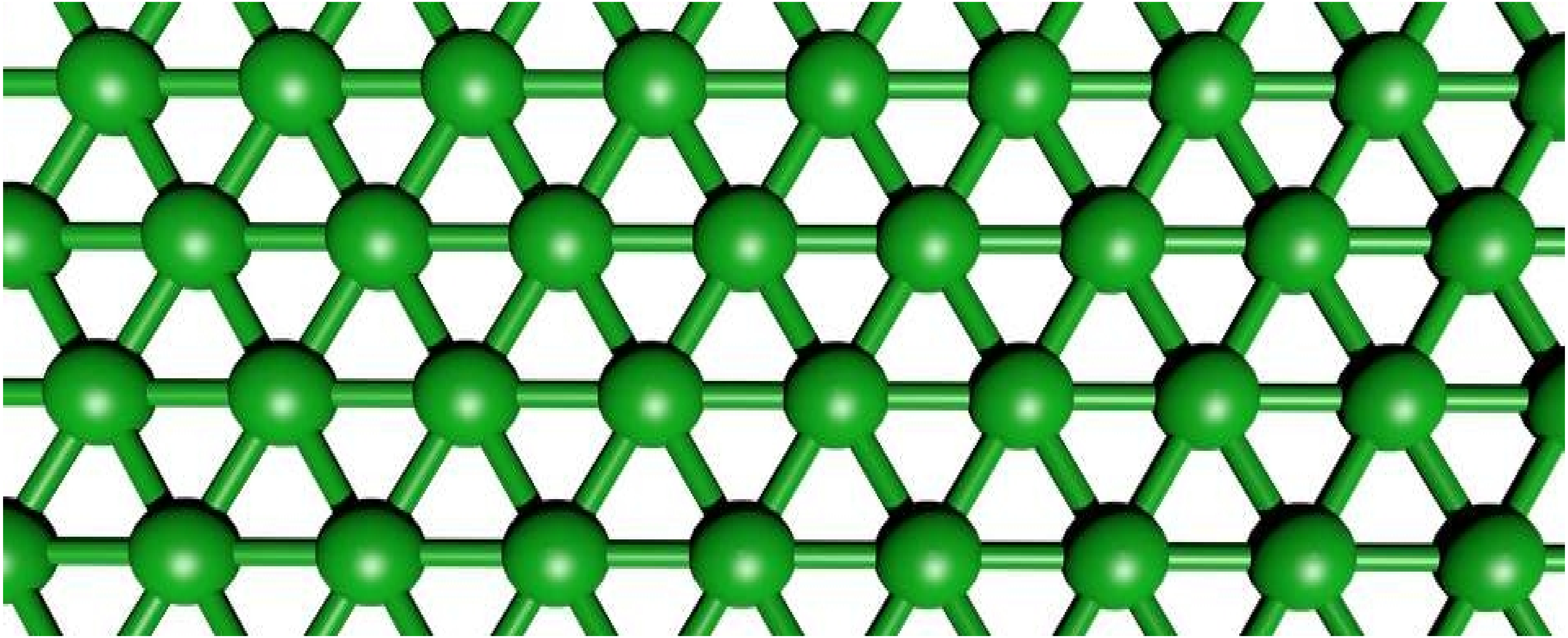


As the rotation angle approached 1 degree, the lowest band becomes flatter

A bilayer van der Waals heterostructure

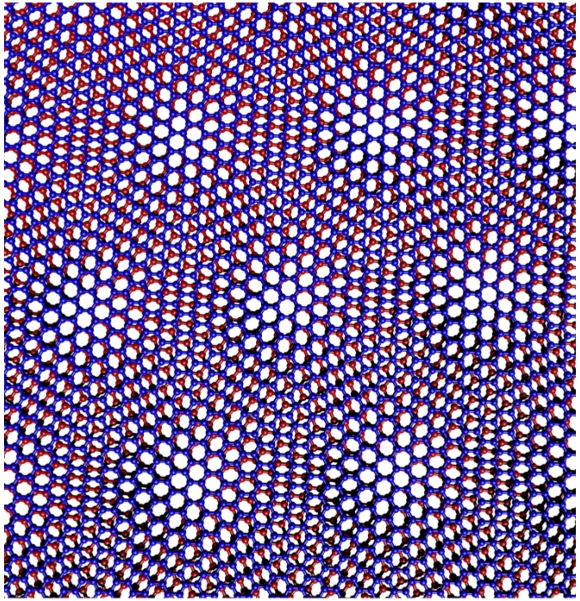


A bilayer van der Waals heterostructure

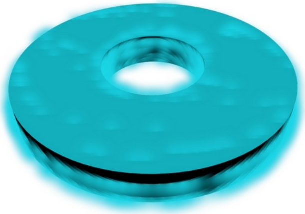


Electronic states in a single moire superlattice

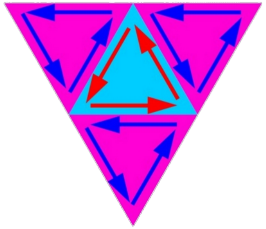
Twisted bilayer graphene



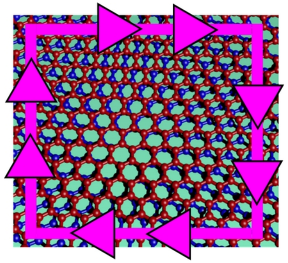
Superconductivity



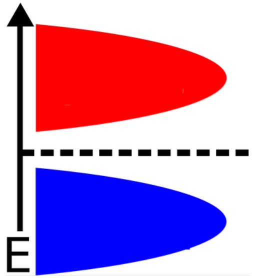
Topological networks



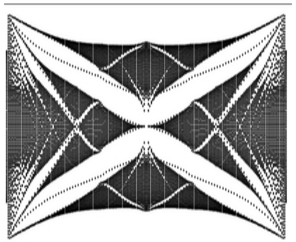
Chern insulators



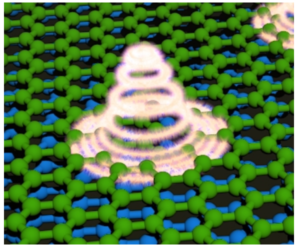
Correlated insulators



Quasicrystalline physics



Fractional Chern insulators



A single twisted van der Waals material realizes a variety of widely different electronic states

Superconductivity, a reminder

A reminder about superconductivity

The original Hamiltonian $$H = \sum_{\mathbf{k},s} \epsilon_{\mathbf{k}} c^\dagger_{\mathbf{k},s} c_{\mathbf{k},s} + \sum_{\mathbf{k}} \Delta c^\dagger_{\mathbf{k},\uparrow} c^\dagger_{-\mathbf{k},\downarrow} + h.c.$$

Can be rewritten as

$$H = \frac{1}{2} \Psi^\dagger_{\mathbf{k}} \mathcal{H} \Psi_{\mathbf{k}}$$

$$\Psi_{\mathbf{k}} = \begin{pmatrix} c_{\mathbf{k}\uparrow} \\ c_{\mathbf{k}\downarrow} \\ c^\dagger_{-\mathbf{k}\downarrow} \\ -c^\dagger_{-\mathbf{k}\uparrow} \end{pmatrix}$$

Electron sector

Hole sector

with $$\mathcal{H} = \begin{pmatrix} \epsilon_{\mathbf{k}} & 0 & \Delta & 0 \\ 0 & \epsilon_{\mathbf{k}} & 0 & \Delta \\ \Delta & 0 & -\epsilon_{\mathbf{k}} & 0 \\ 0 & \Delta & 0 & -\epsilon_{\mathbf{k}} \end{pmatrix}$$

Generic forms of superconductivity

A generic superconducting Hamiltonian

$$\widehat{H}' = \sum_{\boldsymbol{k},\sigma} \epsilon_{\boldsymbol{k}} \, \widehat{c}^{\dagger}_{\boldsymbol{k},\sigma} \, \widehat{c}_{\boldsymbol{k},\sigma} - \frac{1}{2} \sum_{\boldsymbol{k}}{}' \sum_{\sigma_1,\sigma_2} \left[\Delta_{\boldsymbol{k},\sigma_1\sigma_2} \, \widehat{c}^{\dagger}_{\boldsymbol{k},\sigma_1} \, \widehat{c}^{\dagger}_{-\boldsymbol{k},\sigma_2} + \Delta^{*}_{\boldsymbol{k},\sigma_1\sigma_2} \, \widehat{c}_{\boldsymbol{k},\sigma_1} \, \widehat{c}_{-\boldsymbol{k},\sigma_2} \right]$$

Can be characterized by a superconducting matrix

$$\Delta_{\boldsymbol{k}} = \begin{pmatrix} \Delta_{\boldsymbol{k},\uparrow\uparrow} & \Delta_{\boldsymbol{k},\uparrow\downarrow} \\ \Delta_{\boldsymbol{k},\downarrow\uparrow} & \Delta_{\boldsymbol{k},\downarrow\downarrow} \end{pmatrix}$$

The symmetry of the SC order determines the nature of the SC order

Superconducting momentum symmetries

A generic type of a superconductor is characterized by the order parameter

Real space

$$\Delta_{\uparrow\downarrow}(\mathbf{r},\mathbf{r}') \sim \langle c_{\mathbf{r}\uparrow} c_{\mathbf{r}'\downarrow} \rangle$$

Reciprocal space

$$\Delta_{\uparrow\downarrow}(\mathbf{k}) \sim \langle c_{\mathbf{k}\uparrow} c_{-\mathbf{k}\downarrow} \rangle$$

The superconducting state can be characterized by the symmetry of $\Delta_{\uparrow\downarrow}(\mathbf{k})$

Singlet and triplet superconductors

The superconducting order inherits a symmetry property

$$\Delta_{\vec{k},s_1 s_2} = -\Delta_{-\vec{k},s_2 s_1} = \begin{cases} \Delta_{-\vec{k},s_1 s_2} = -\Delta_{\vec{k},s_2 s_1} & \text{even} \\ -\Delta_{-\vec{k},s_1 s_2} = \Delta_{\vec{k},s_2 s_1} & \text{odd} \end{cases}$$

Spin-singlet (even)

$$\Delta_{\uparrow\downarrow}(\mathbf{k}) = \Delta_{\uparrow\downarrow}(-\mathbf{k})$$

Spin-triplet (odd)

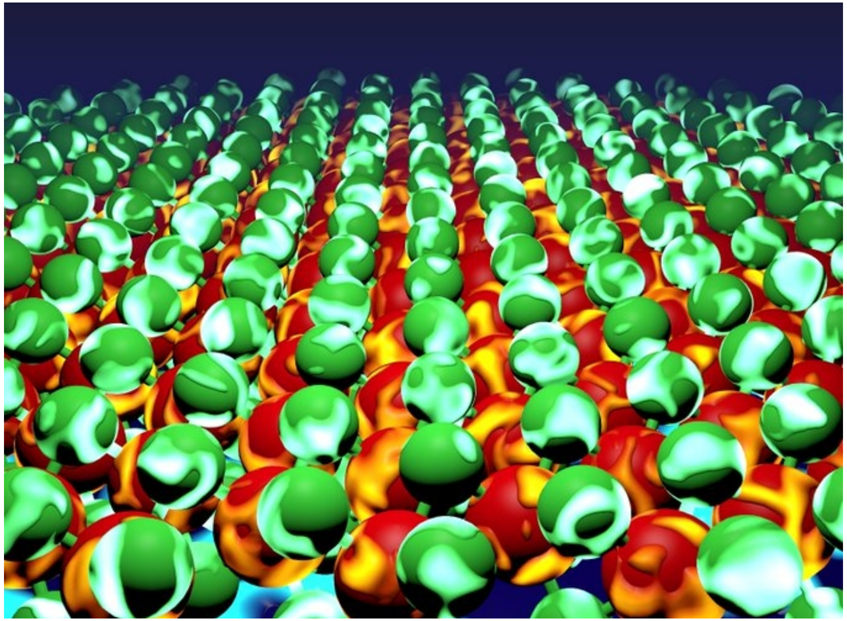
$$\Delta_{\uparrow\uparrow}(\mathbf{k}) = -\Delta_{\uparrow\uparrow}(-\mathbf{k})$$

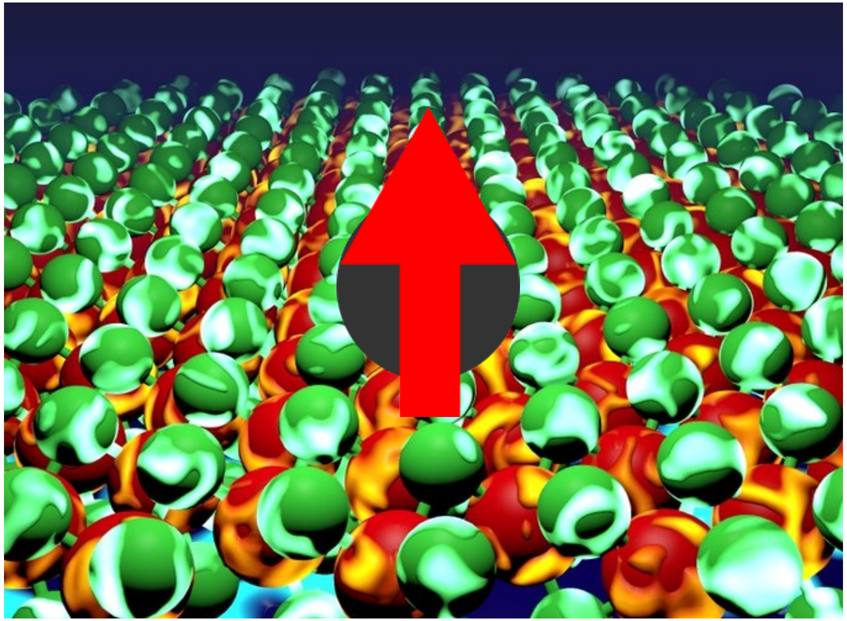
The symmetry of the superconducting order characterizes the superconductor

Superconductivity and magnetism

Impurities in 2D superconductors

What happens if you simulataneously superconductivity and a magnetic impurity?

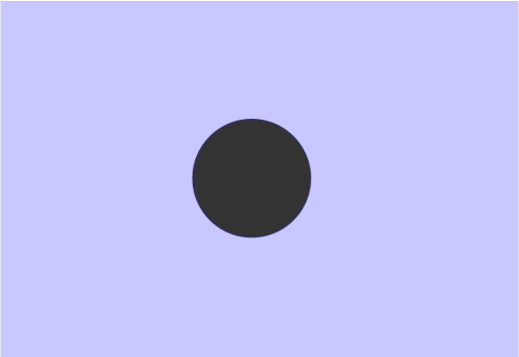




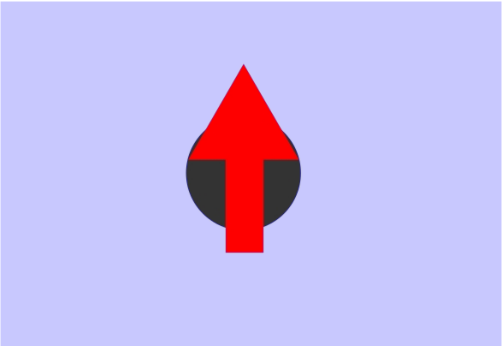
How detrimental are defects in superconductors?

Impurities in 2D superconductors

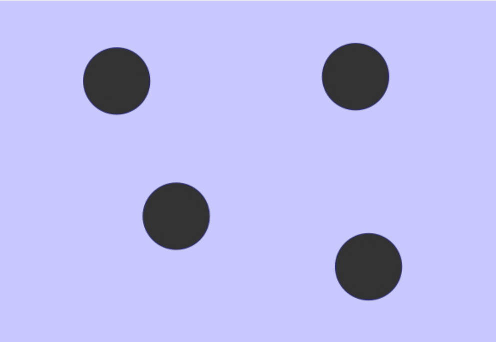
A non-magnetic impurity



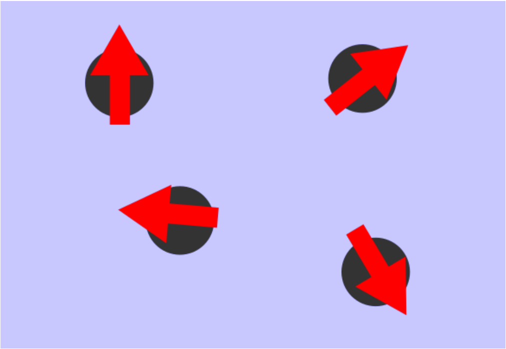
A magnetic impurity



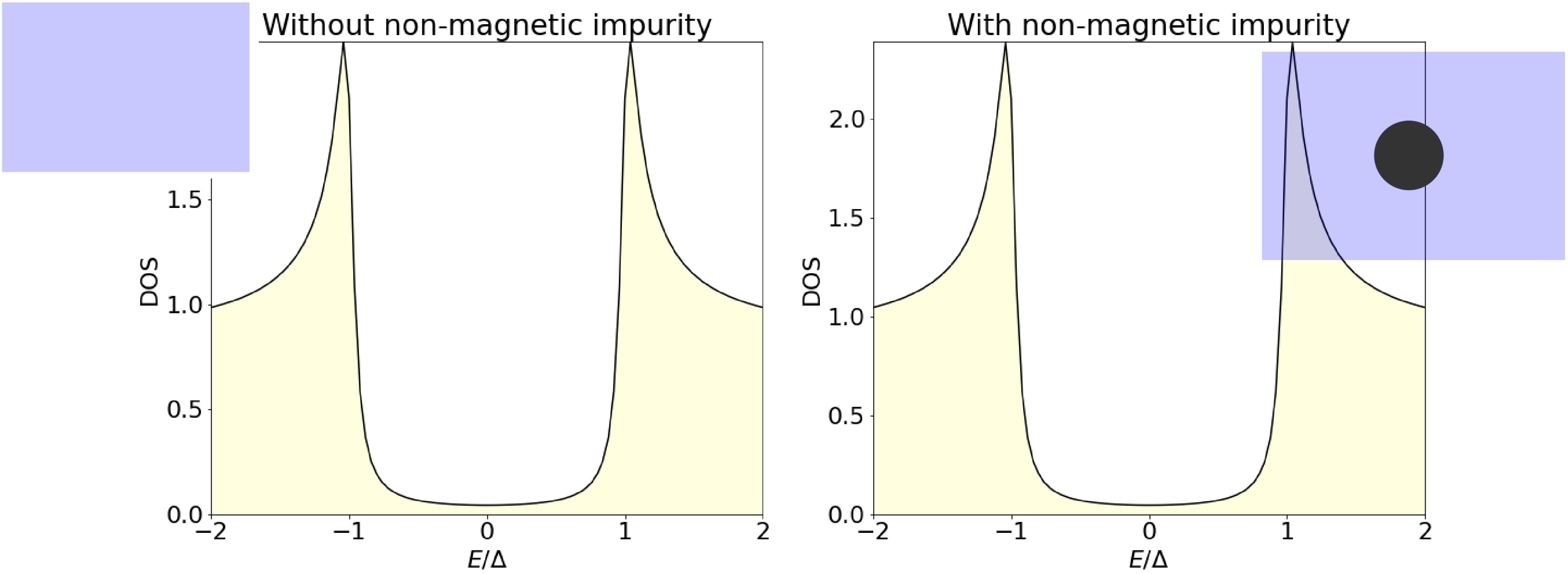
Several non-magnetic impurities



Several magnetic impurities

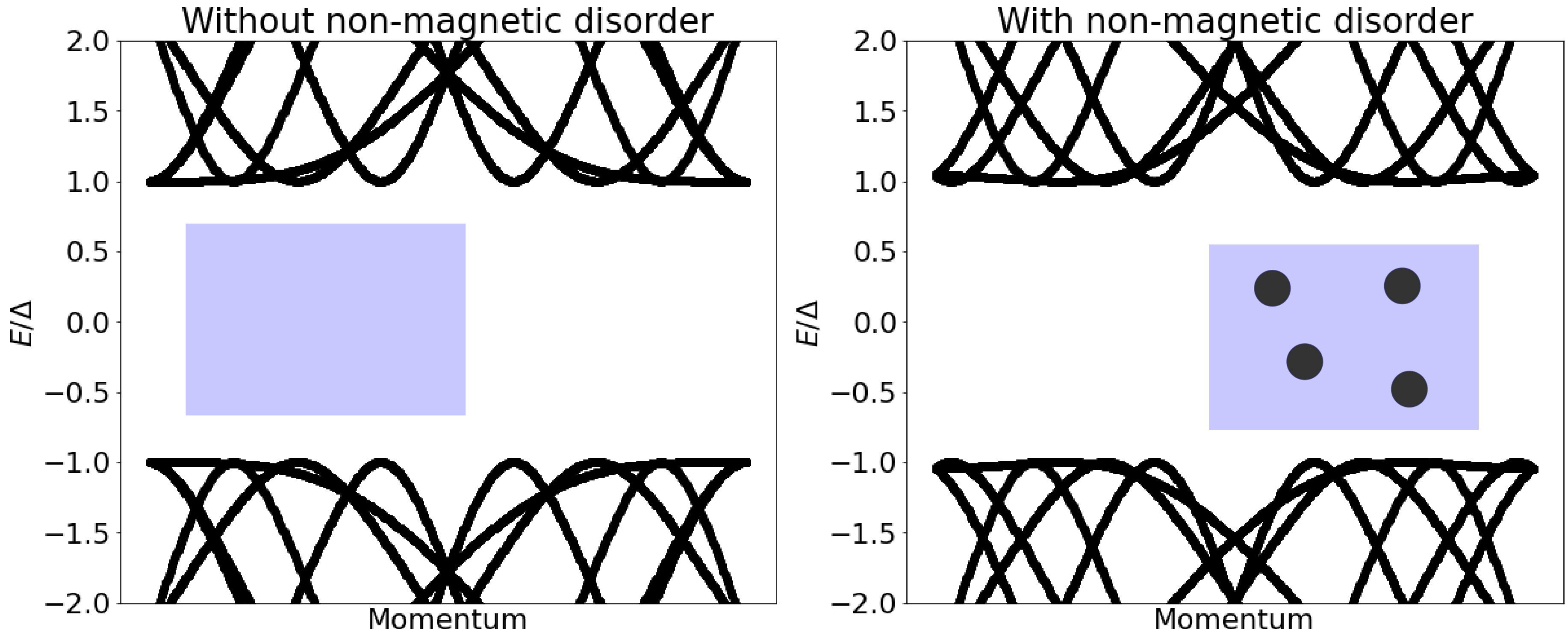


Non-magnetic impurity, conventional s-wave superconductor



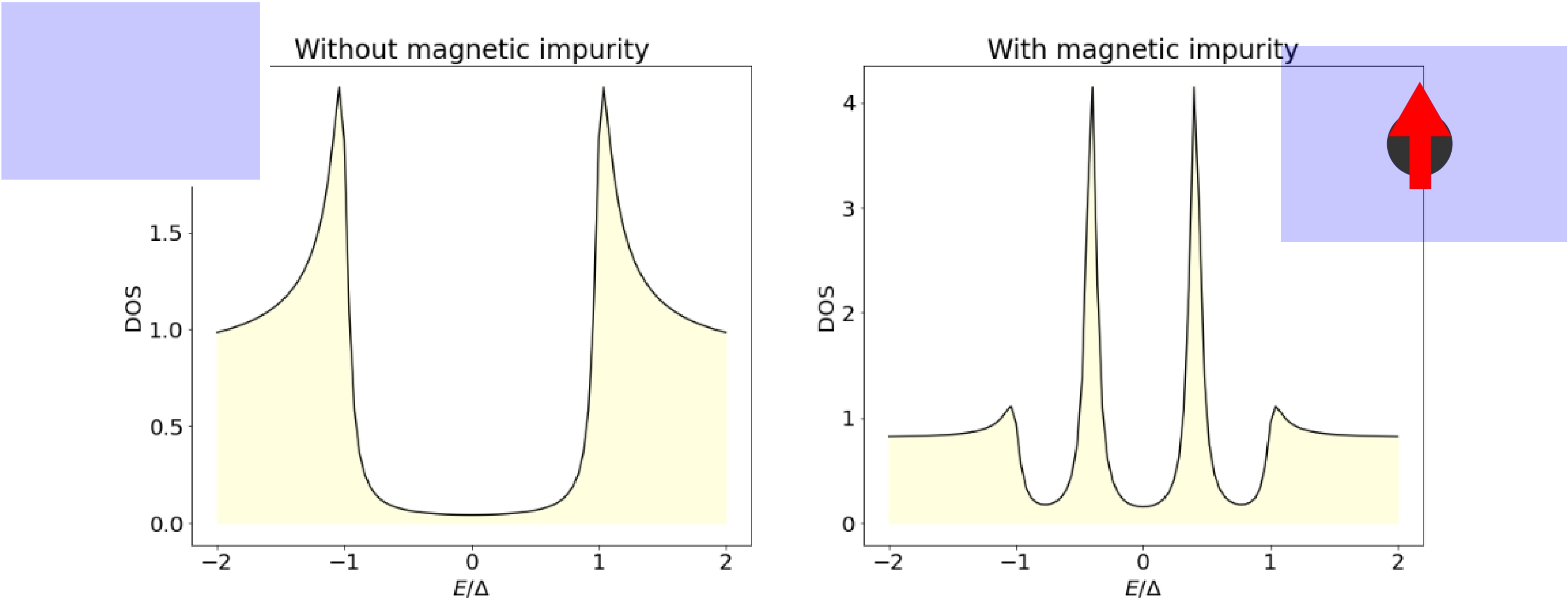
A non-magnetic impurity does not affect conventional s-wave superconductors

Non-magnetic disorder, conventional s-wave superconductor



Non-magnetic disorder does not impact a conventional s-wave superconducting gap

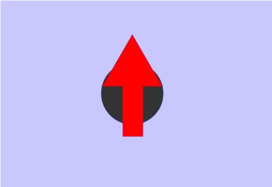
The interplay between magnetism and superconductivity

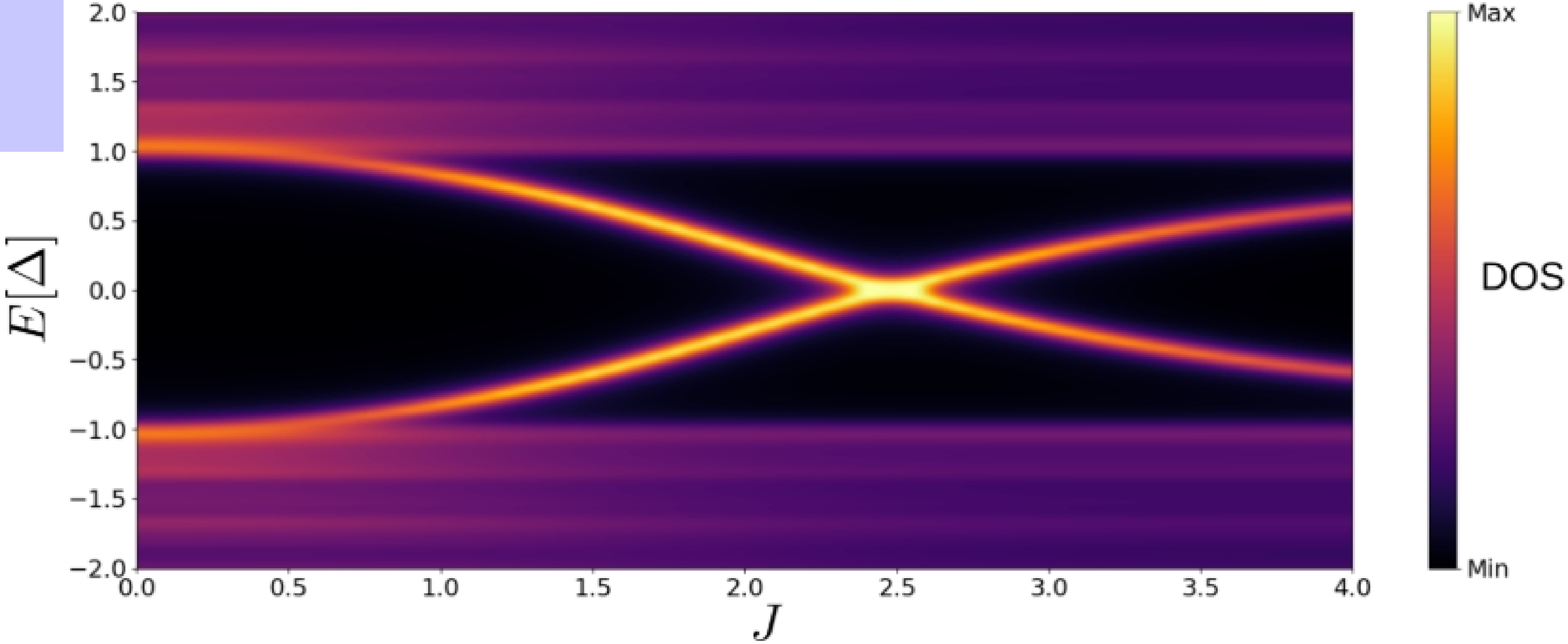


Magnetic impurities create in-gap states in fully gapped superconductors

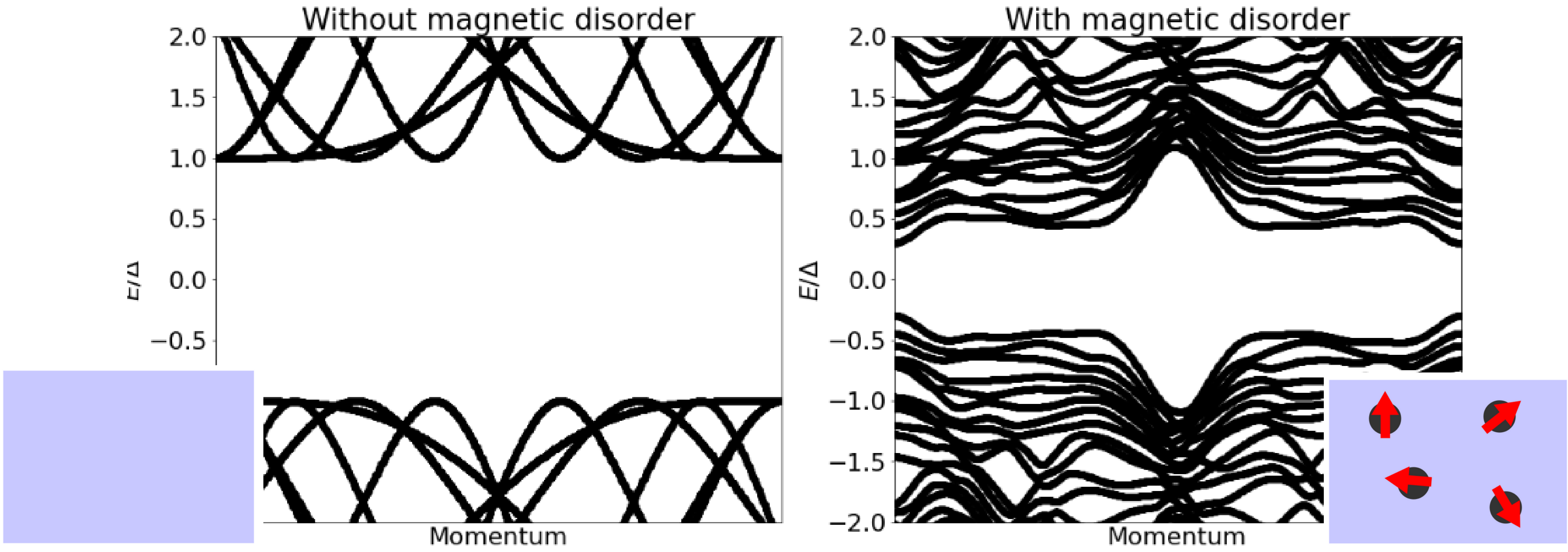
The interplay between magnetism and superconductivity

The exchange coupling controls the energy of the in-gap state



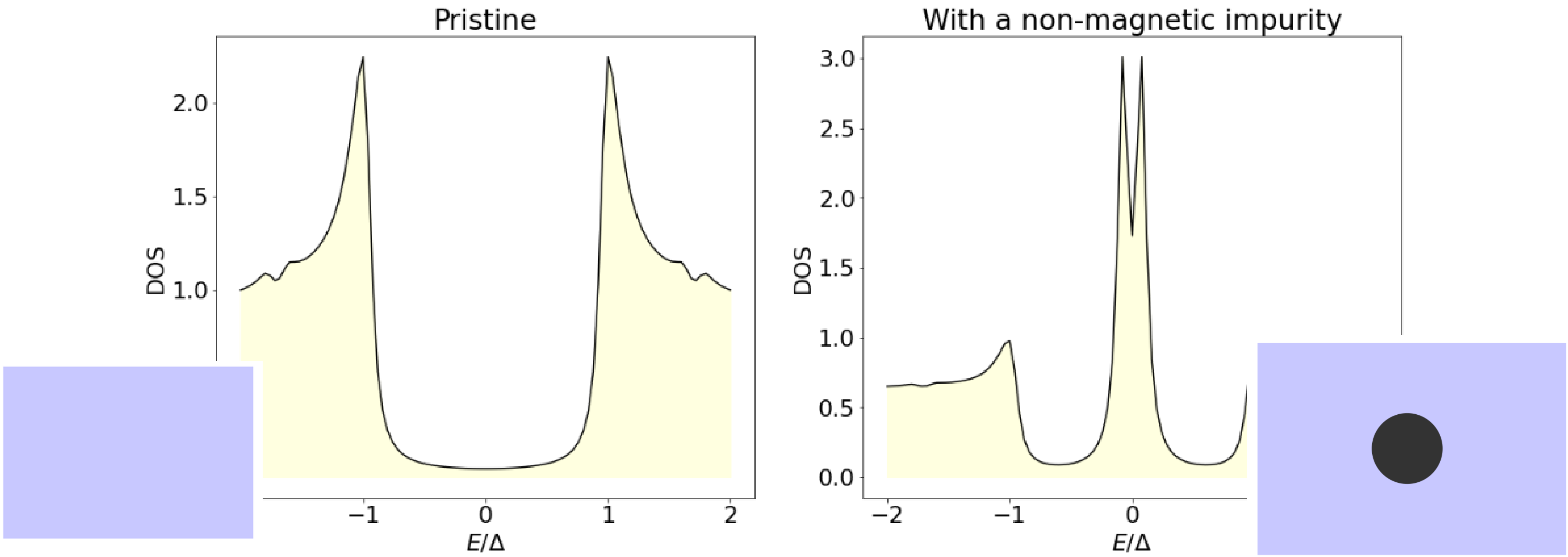


The effect of magnetic disorder in superconductors



Magnetic disorder decreases the gap of conventional superconductors

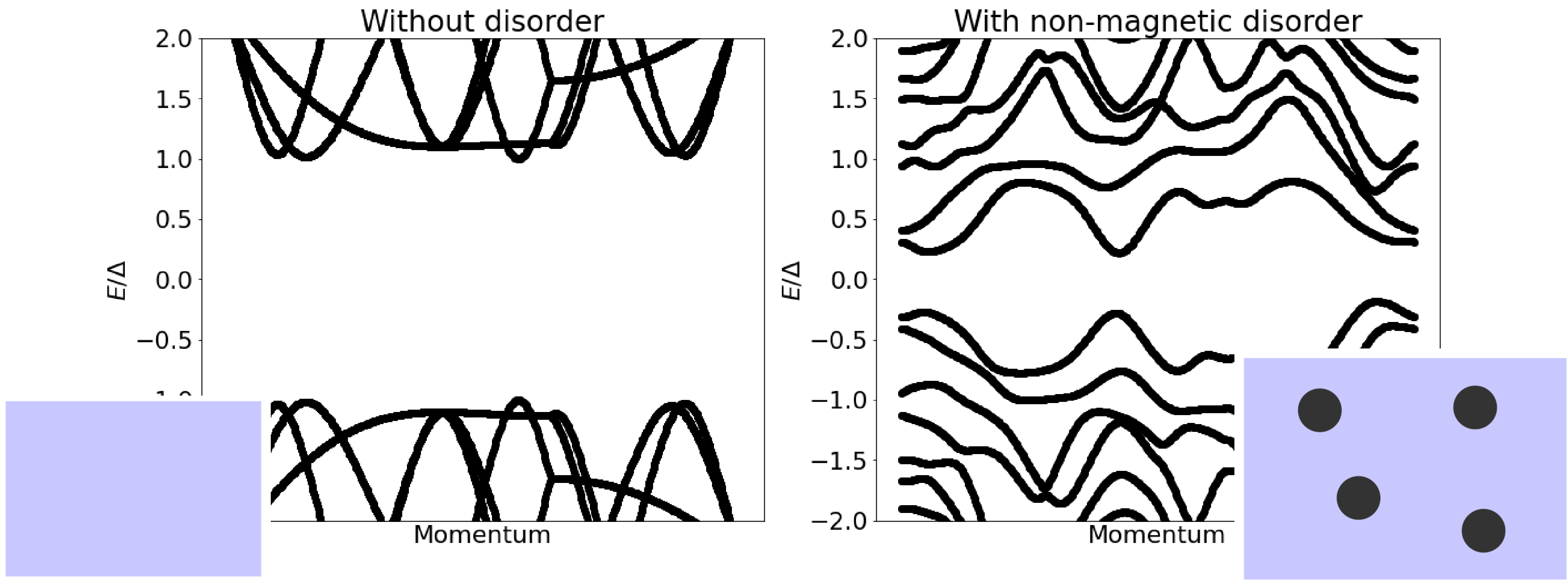
The interplay between impurities and unconventional superconductivity



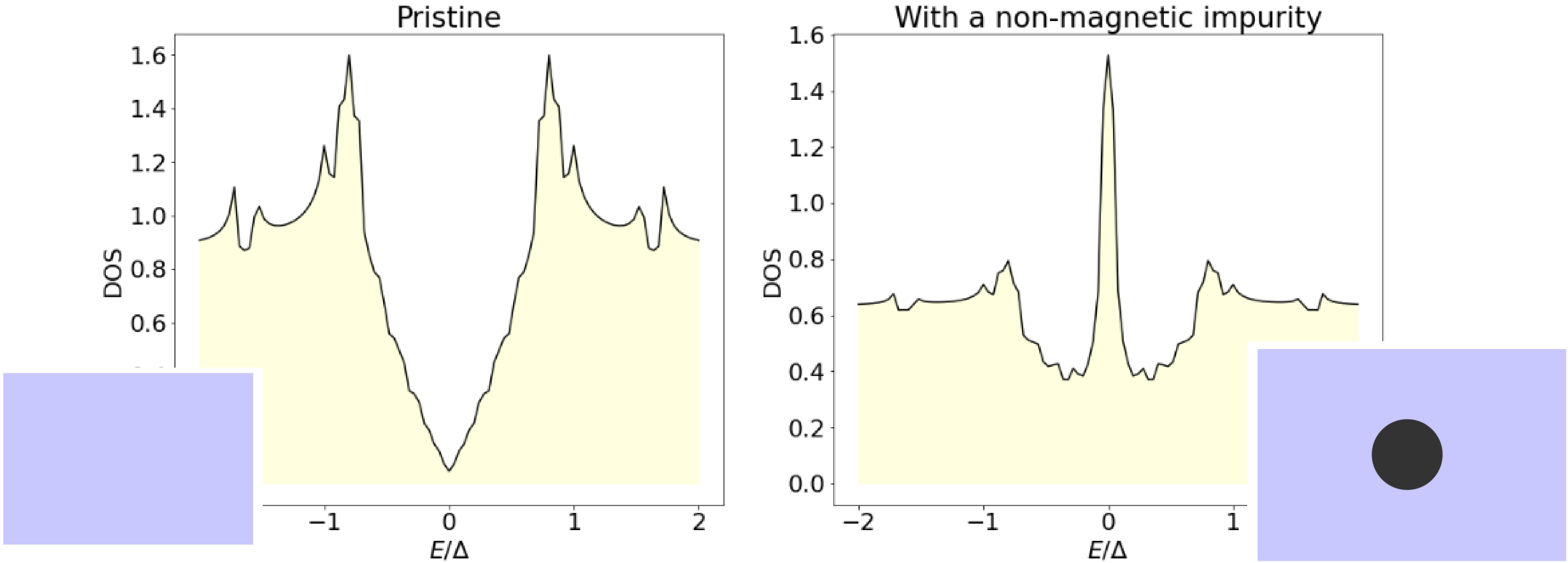
Non-magnetic impurities create in-gap states in fully gapped unconventional superconductors

The impact of non-magnetic disorder in unconventional superconductors

Non-magnetic disorder in unconventional superconductors decreases the gap



Non-magnetic impurities in nodal superconductors



Non-magnetic impurities create in-gap states in nodal unconventional superconductors

A short question

To discuss

What type of superconducting order is each one?

$$c^{\dagger}_{n,\uparrow}c^{\dagger}_{n,\downarrow} \qquad c^{\dagger}_{n,\uparrow}c^{\dagger}_{n+1,\downarrow} \qquad c^{\dagger}_{n,\uparrow}c^{\dagger}_{n+1,\uparrow}$$

and which symmetries do they break?

Topology, a reminder

Topological invariant in a Hamiltonian

We can classify Hamiltonians according to topological invariants

Hamiltonian

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

Wavefunction

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

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

Metric
(Berry curvature)

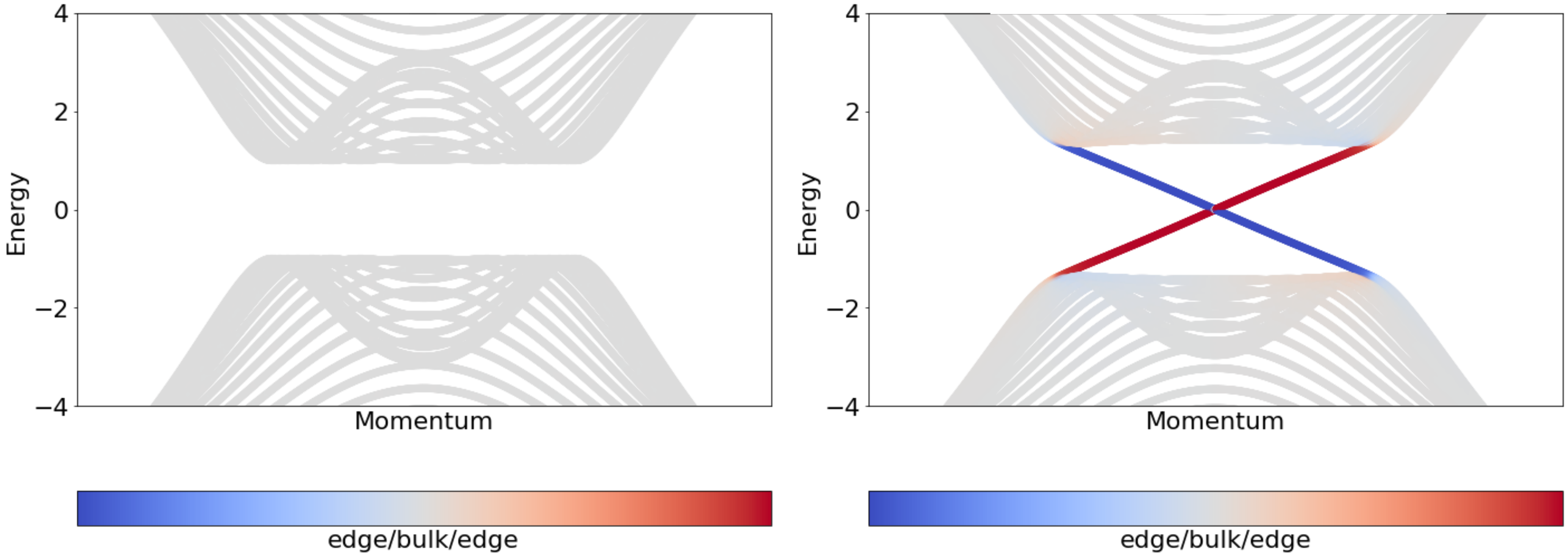
$$C = \int_{BZ} \Omega d^2\mathbf{k}$$

Topological invariant
(Chern number)

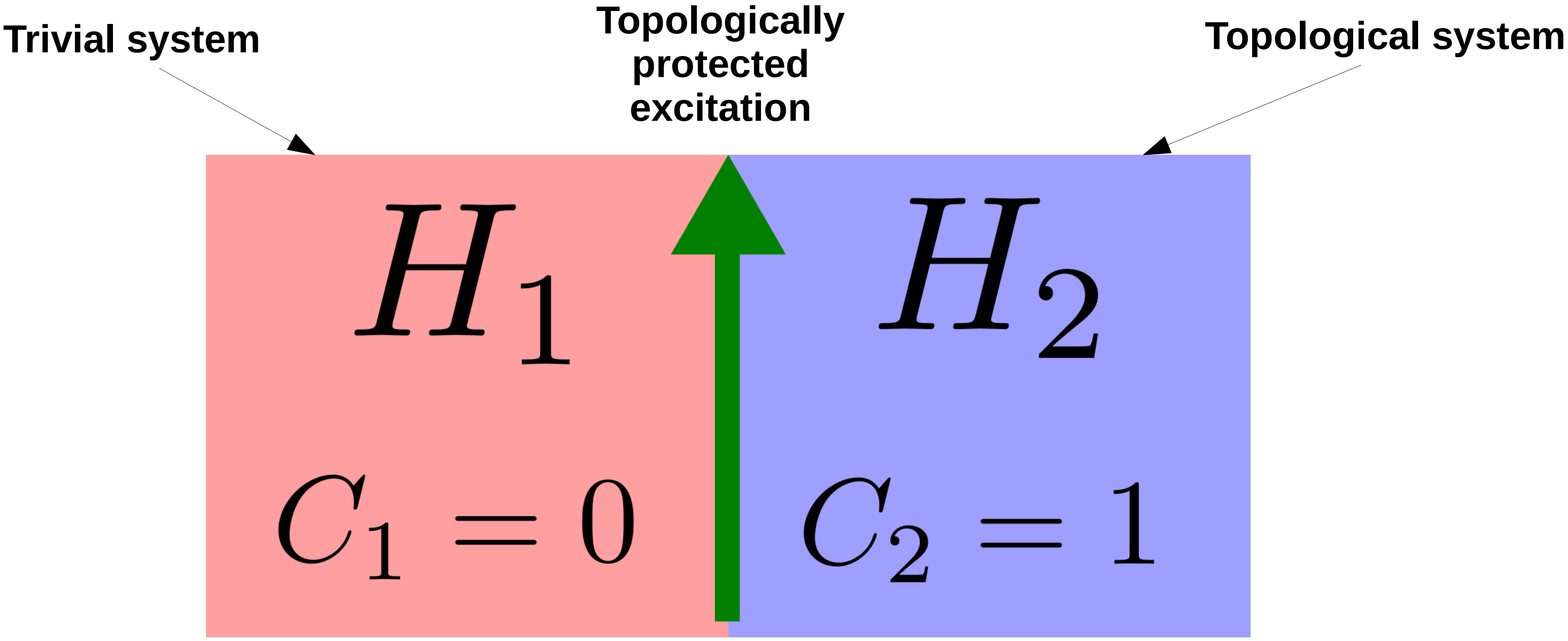
The role of a topological invariant

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

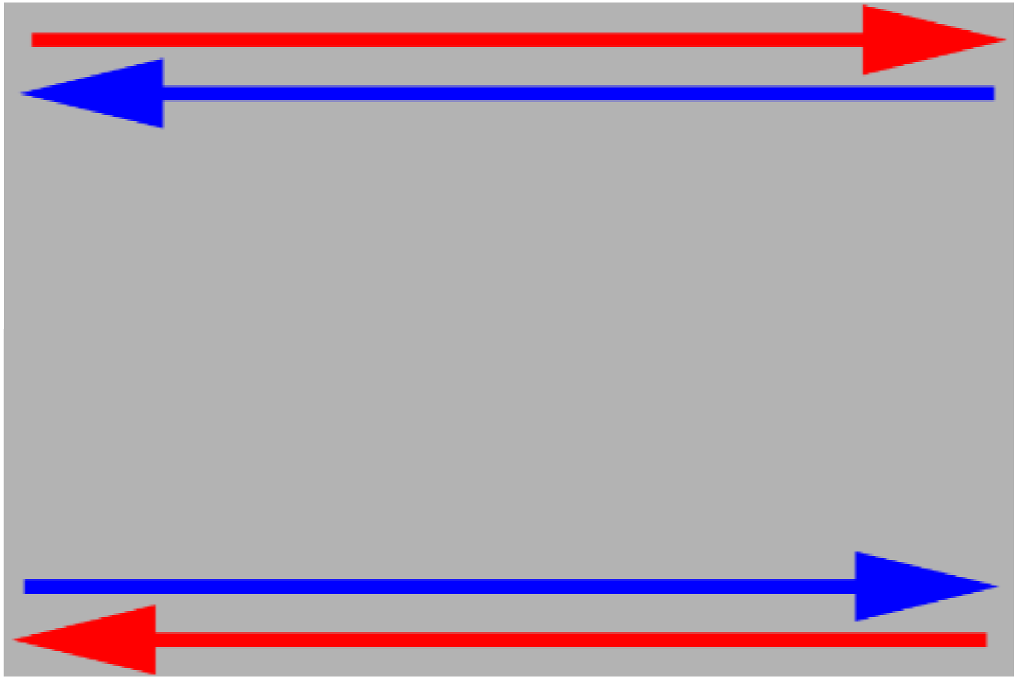


Topological excitations appear between topologically different systems

Topology from Dirac equations

Edge states in quantum spin Hall insulators

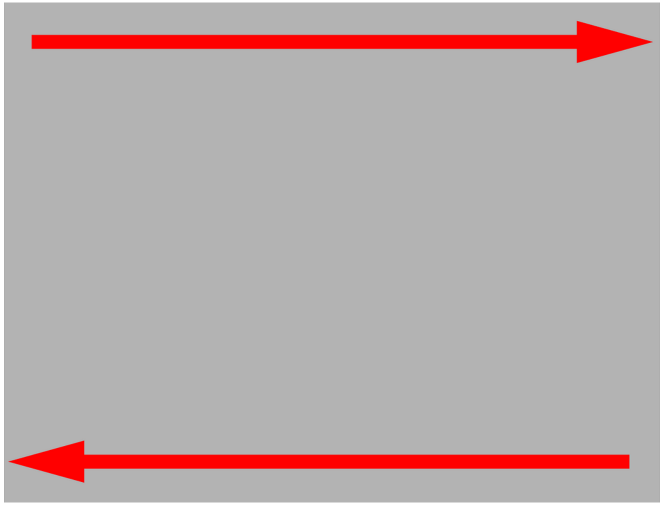
In a quantum spin Hall insulator, opposite spin propagate in opposite directions



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

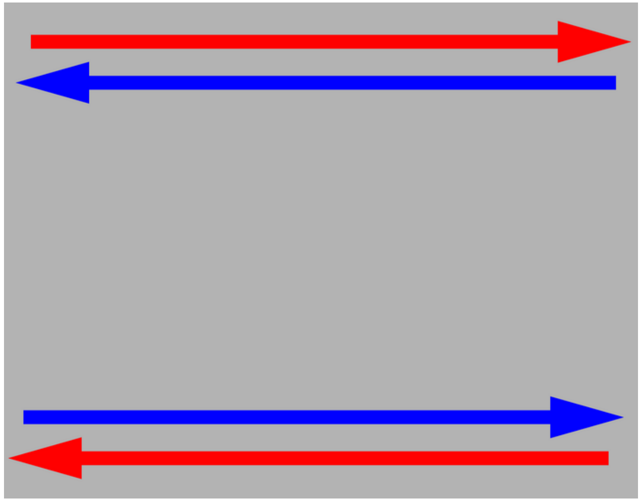
The relation between two topological states

Chern insulators



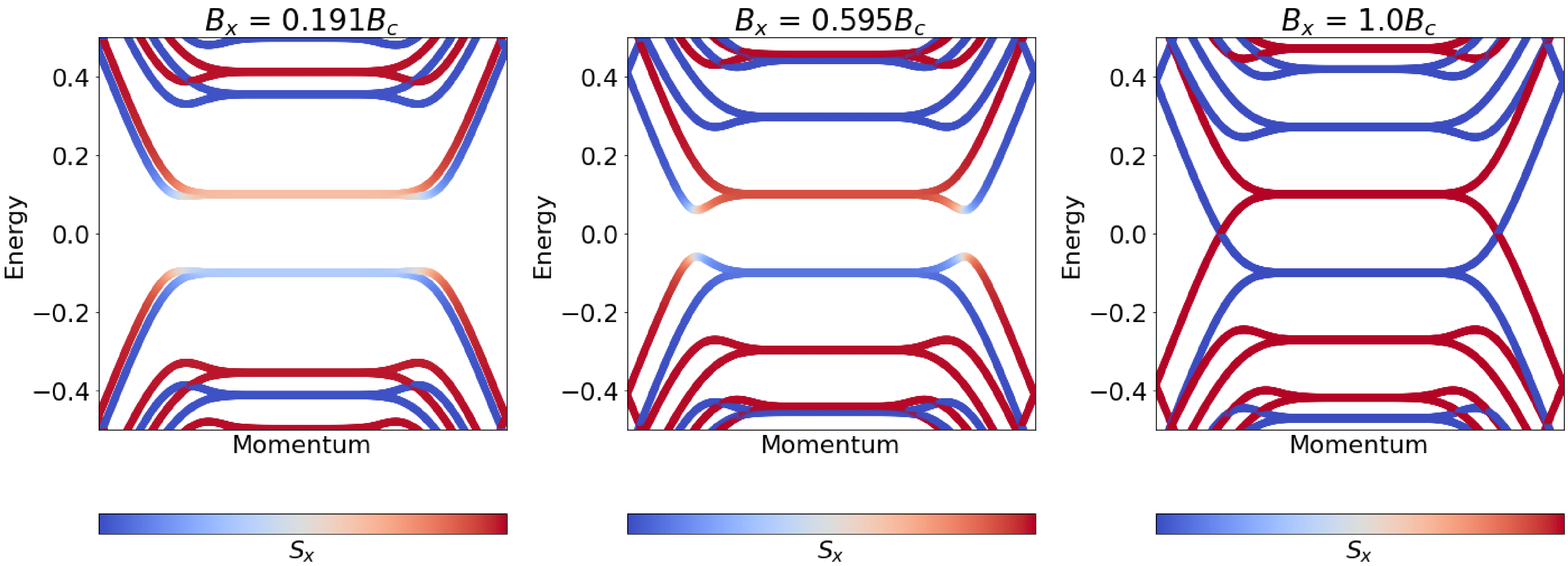
Chiral modes
Break time-reversal symmetry

Quantum spin Hall insulators



Helical modes
Do not break time-reversal symmetry

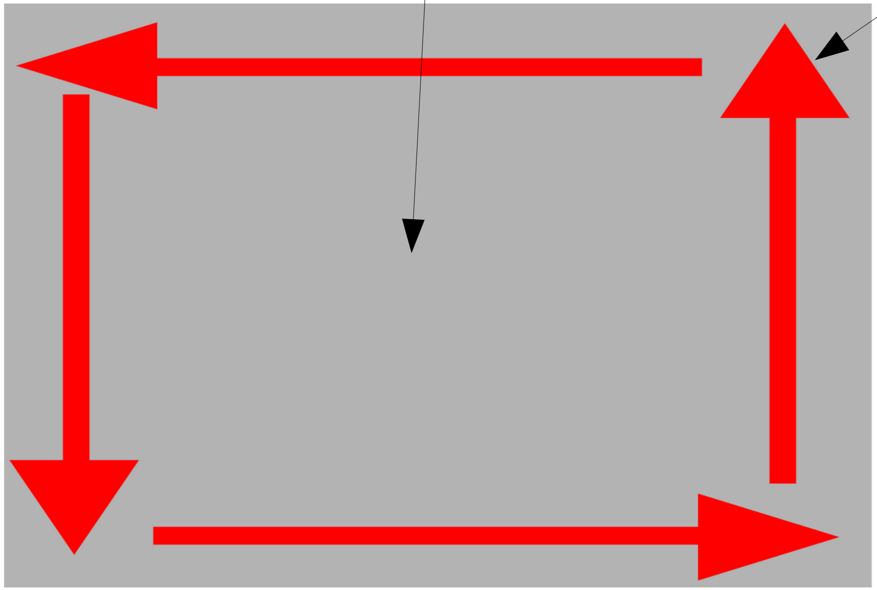
The quantum spin Hall state driven by magnetic field in graphene



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)

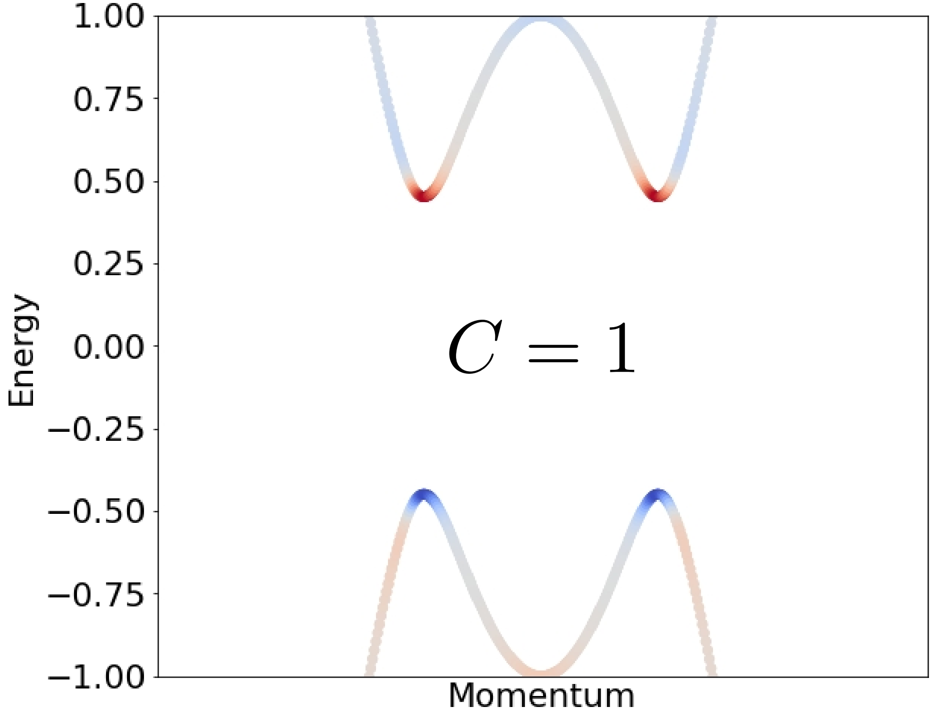
Hall conductivity (Chern number)

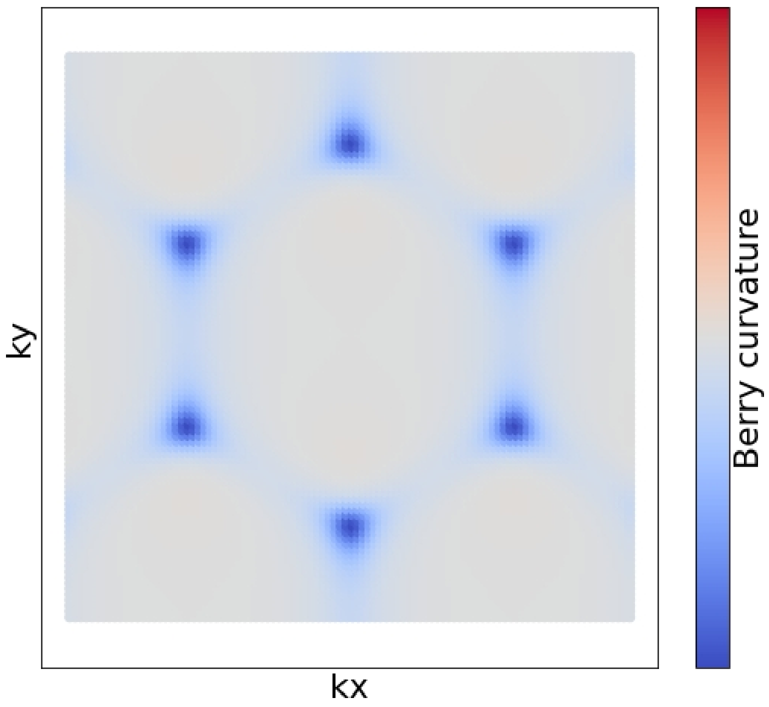
$$\sigma_{xy} = \sum_{\alpha \in occ} \int \Omega_\alpha d^2\mathbf{k} = \sum_\alpha C_\alpha = C$$

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

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

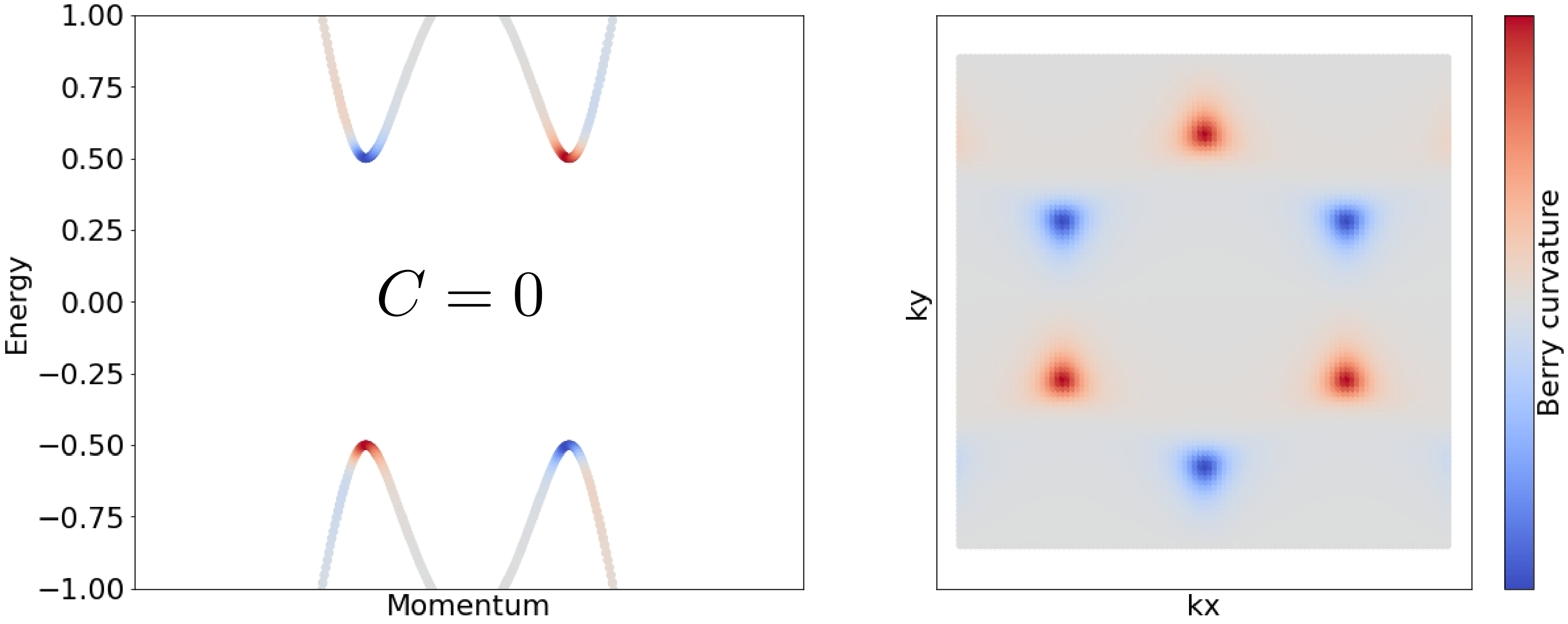
Two different gaps in a 2D material





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

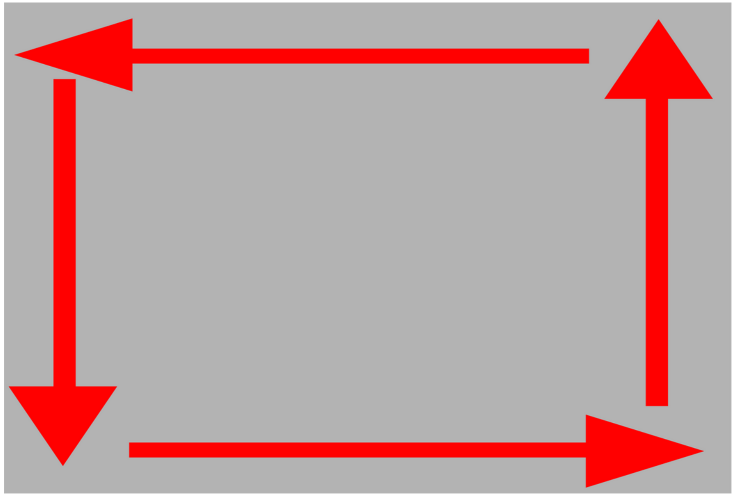
$$C_S = C_\uparrow - C_\downarrow = \pm 2$$

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

Quantum spin Hall insulators

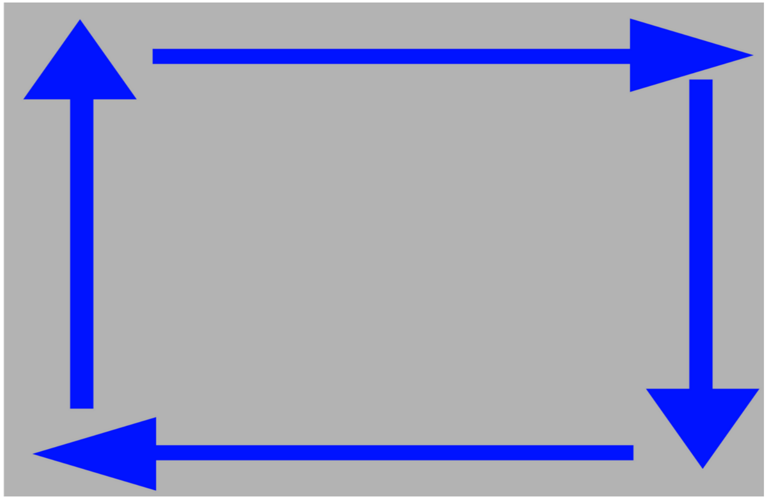
Chern insulator for spin up

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



Chern insulator for spin down

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



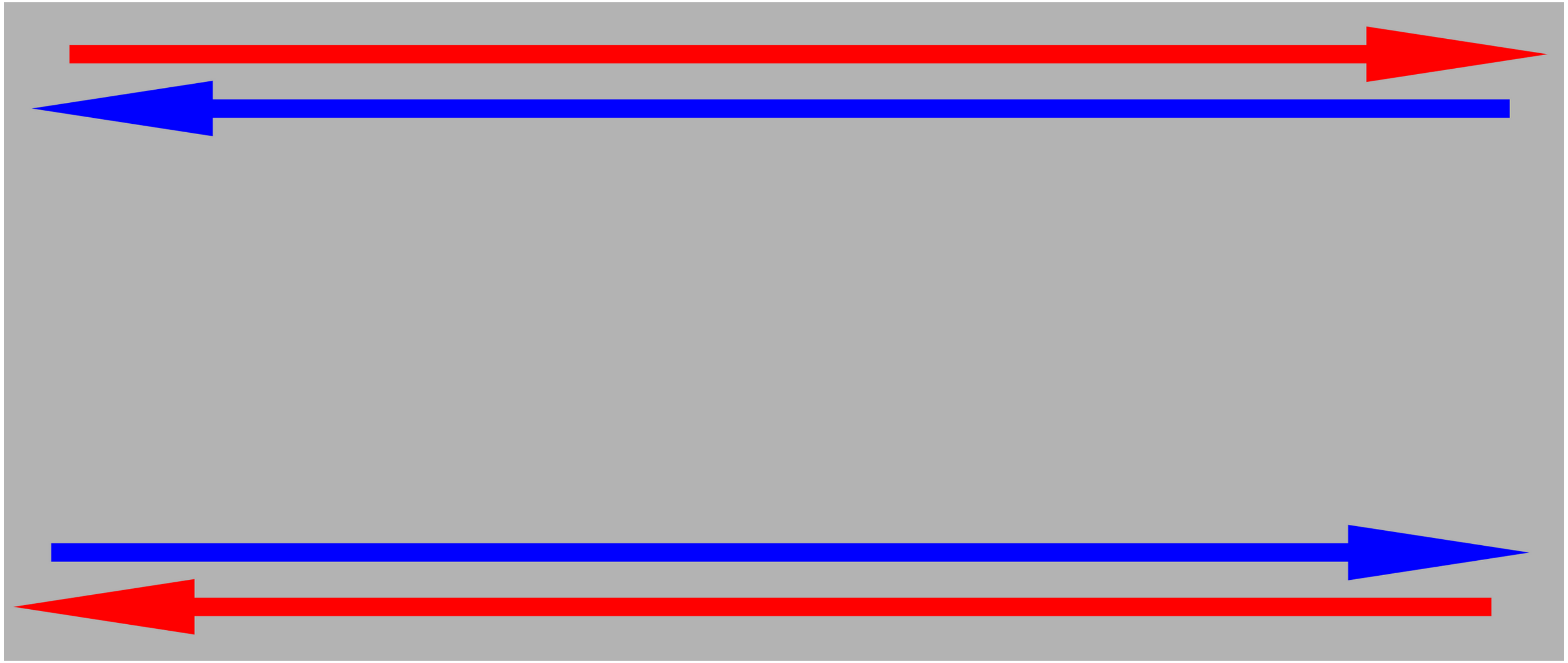
Spin-orbit coupling (SOC) can drive a quantum spin Hall state

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

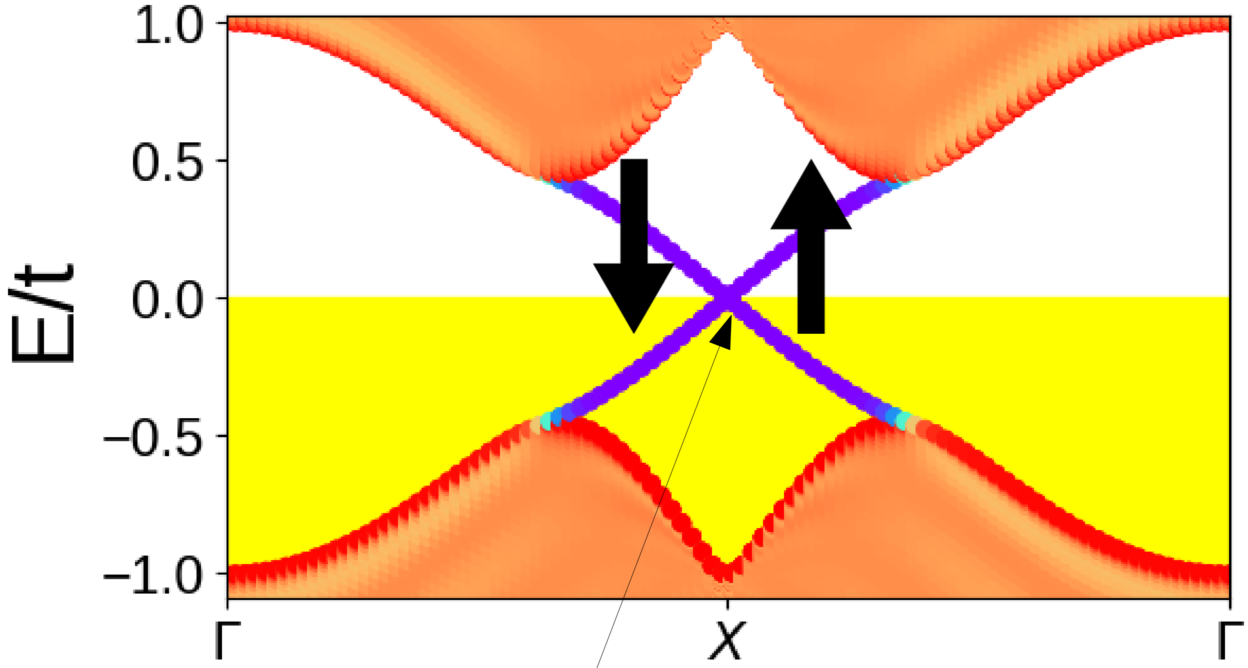
SOC acts as a magnetic field with opposite signs for opposite spins

Quantum spin Hall insulators

Opposite spins propagate in opposite directions (helical gas)



Quantum spin Hall insulators

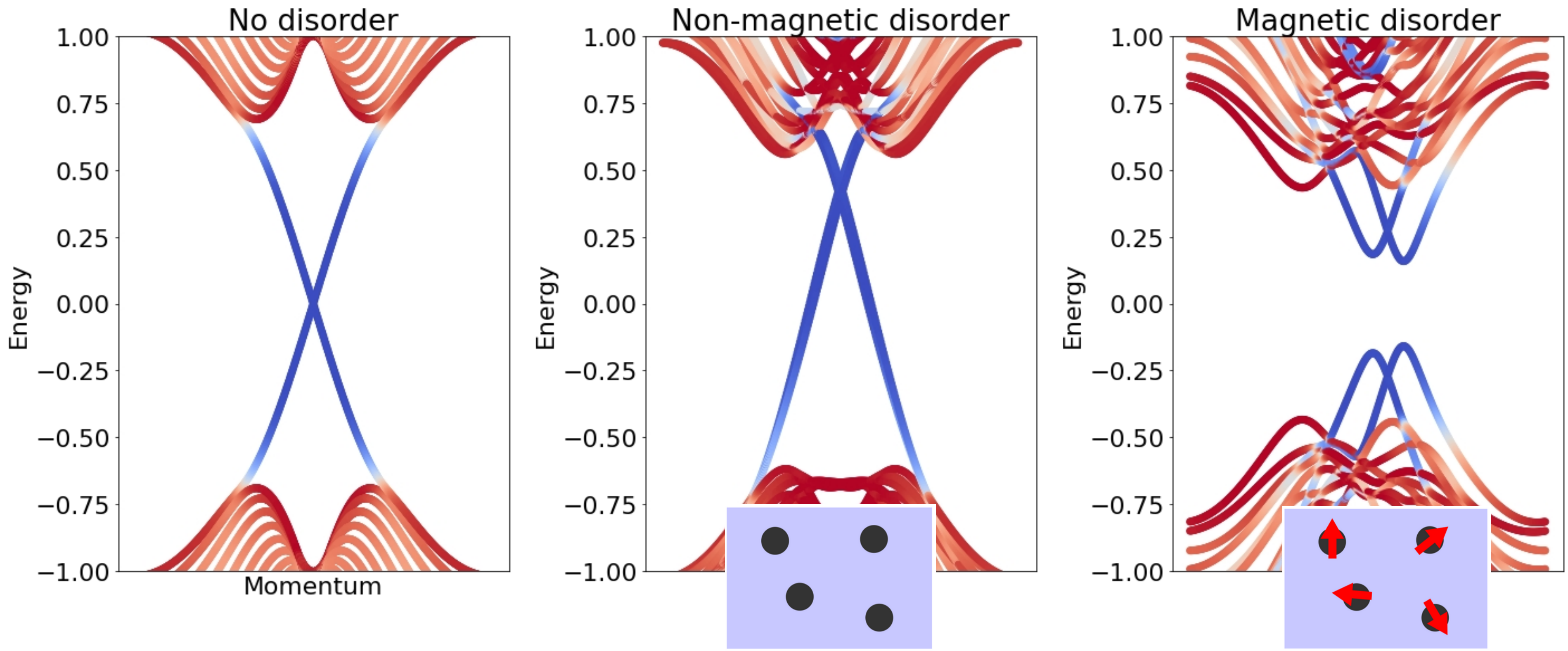


The gapless nature is protected by Kramer’s theorem

Time-reversal symmetry

$$\Theta^2 = -1$$

Disorder in quantum spin Hall insulators

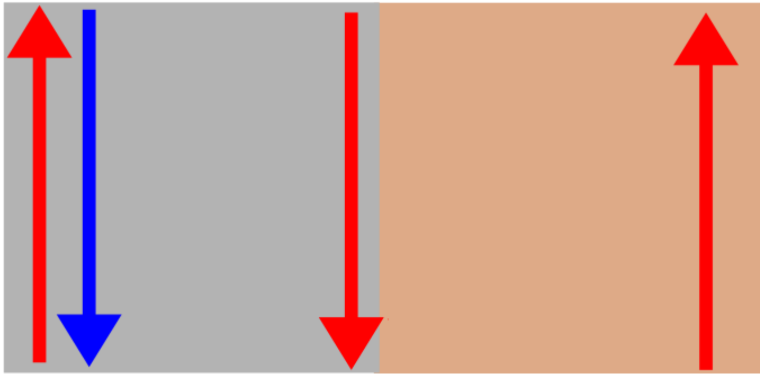


Disorder that breaks time reversal symmetry opens a gap in the topological states

A short question

To discuss

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



Summary

Thank you for joining the course