Chair of Experimental Solid State Physics, LMU Munich

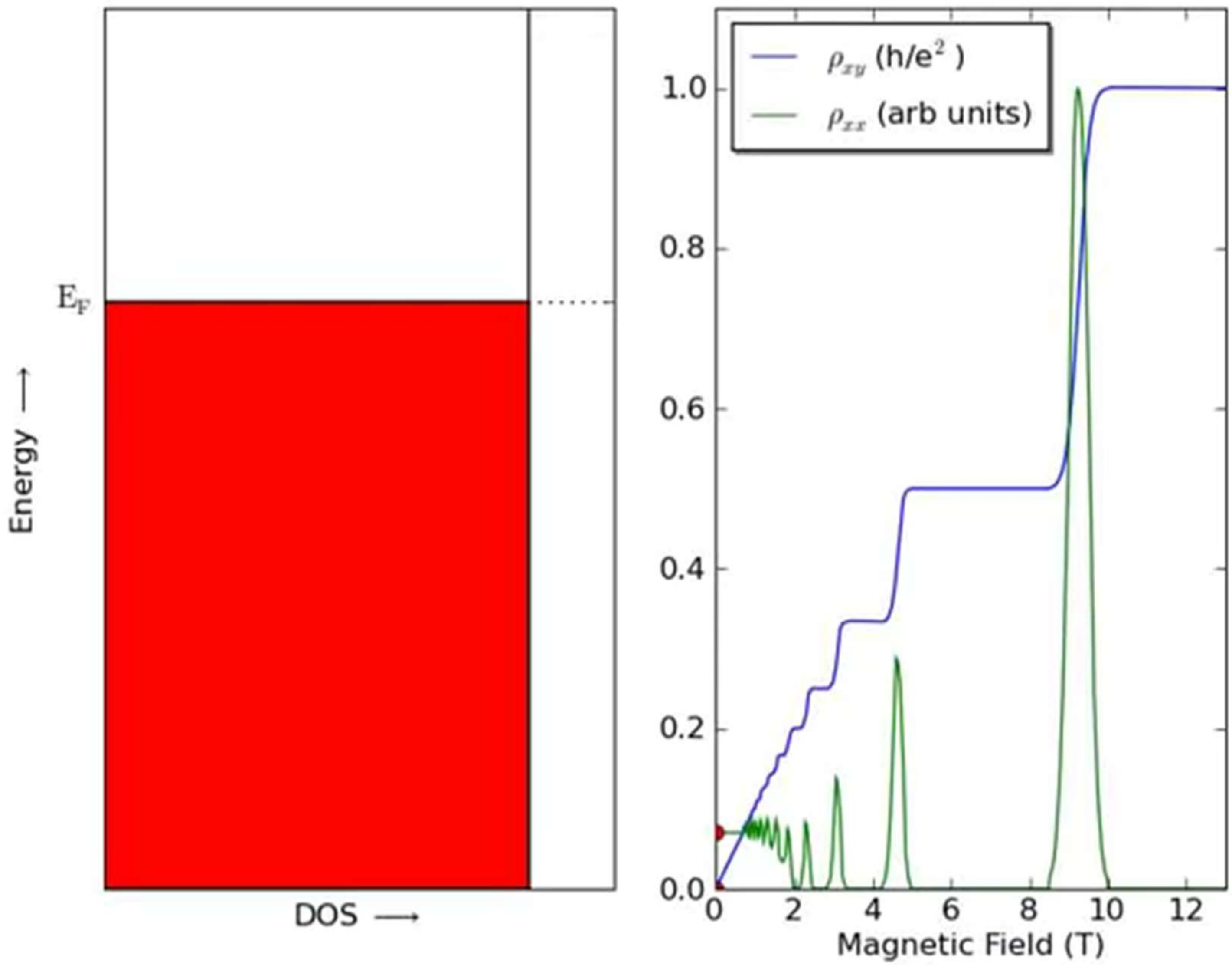
“Introduction to Graphene and 2D Materials”

SS24 Lecture 8, 10/06/2024

Outline - Lecture 8

- Reminder about the QHE effect and occurrence of 1D edge states.
- New types of topological order defined by topological invariants.
- Berry's phase.
- Example of occurrence of the Berry's phase in graphene QHE.
- Haldane model - Graphene-like model as starting point for topologically non-trivial phases.
- Topological insulators - new class of topological phases in zero magnetic field.

Linking filling of the LLs with transport measurements



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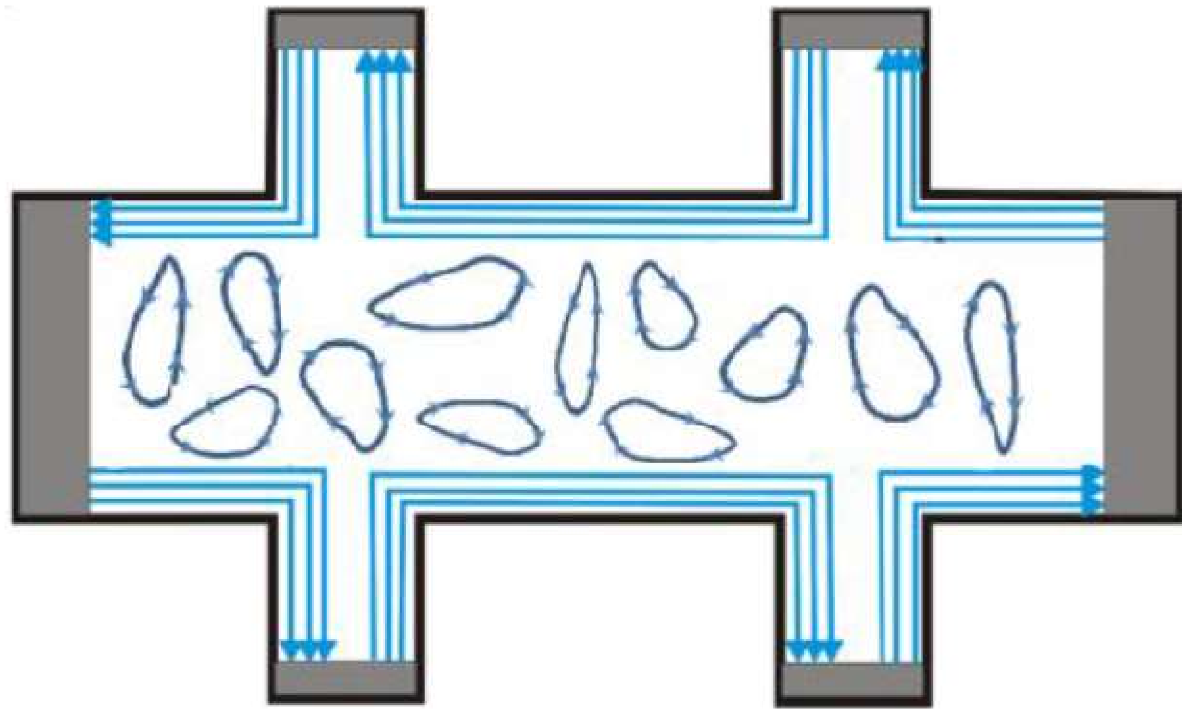
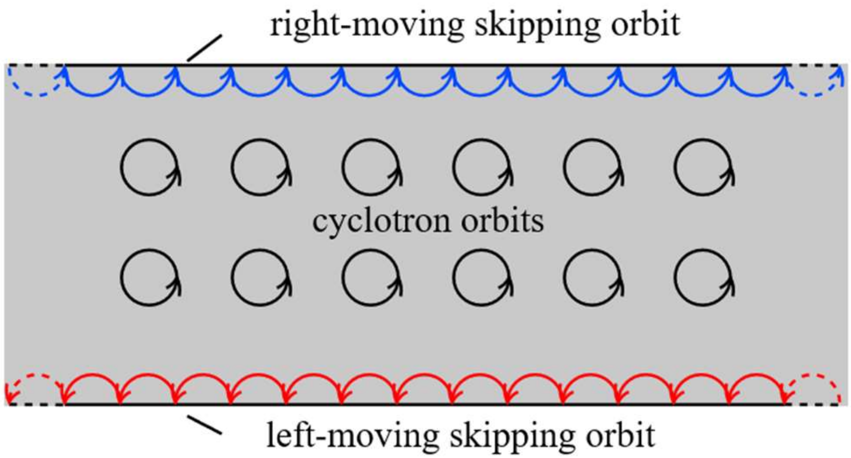
QHE – delocalized chiral 1D edge states



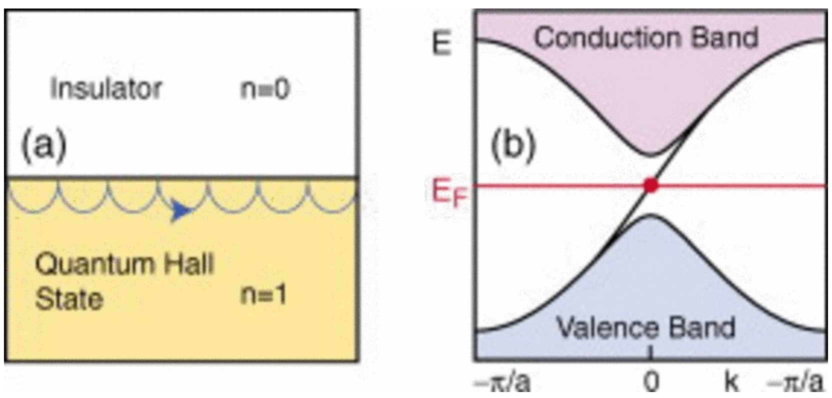
- Formation of chiral 1D edge states at the edges of the device.
- These states represent a novel order and ground states of matter.
- They are topologically protected and their exact quantization $R_{xy} = (h/e^2)/\nu$ follows from this protection (here $\nu = 3$).
- Number of edge states = Chern number (here C = +3, where + is clockwise and – is counterclockwise motion)

Topologically protected edge and localized bulk states

Schematic of a Quantum Hall State:



Band-diagram of edge states:



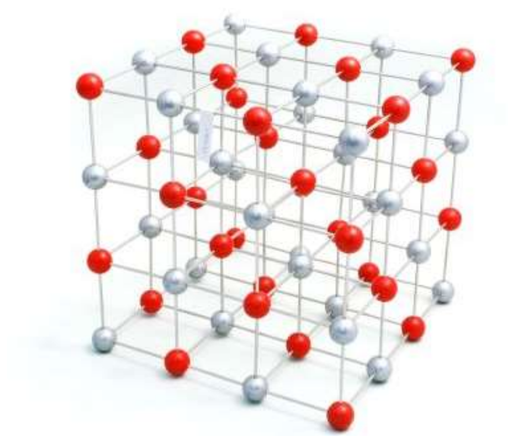
- Orbital states in the bulk are localized → bulk is insulating and a mobility gap is formed (Anderson localization).
- 1D edge states moving in one direction are formed at the edge → these are topologically protected, as back-scattering is not allowed, resulting in perfectly quantized and dissipation-less states.
- Symmetry protected topological states → a topological invariant protects these states and their quantization.

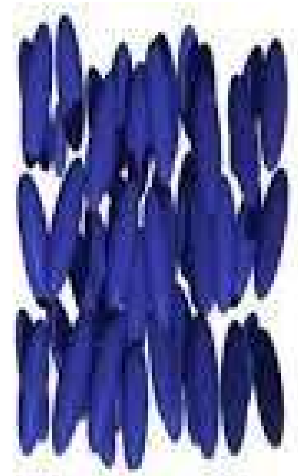
Types of order

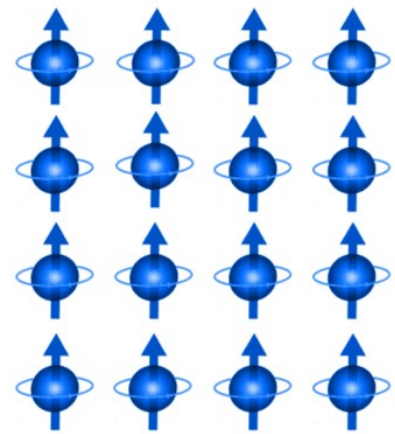
- Most of condensed matter physics is about how different kinds of **order** emerge from interaction between many simple constituents.

- Until 1980, all ordered phases could be understood being due to some sort of “symmetry breaking”

  → An ordered state appears at low temperatures when the system spontaneously loses one of symmetries present at high temperature and establishes a well-defined order parameter.







Examples:

- Crystals → break the **translation and rotation symmetries** of free space.

- Liquid crystals → break **rotational but not translational** symmetry.

- Magnets → break **time-reversal symmetry** and the **rotational symmetry of spin space**.

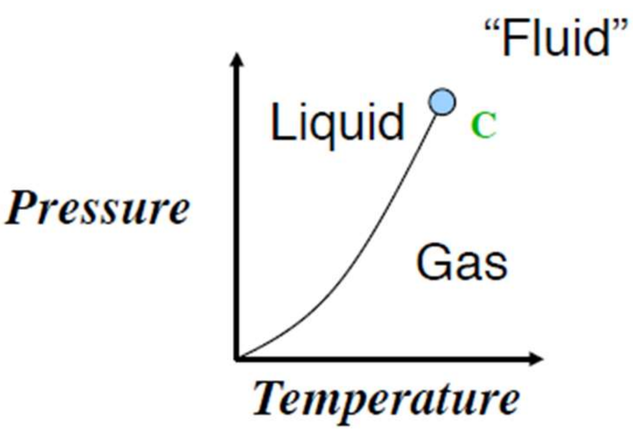
- Superfluids → break an **internal symmetry of quantum mechanics**.

Types of order

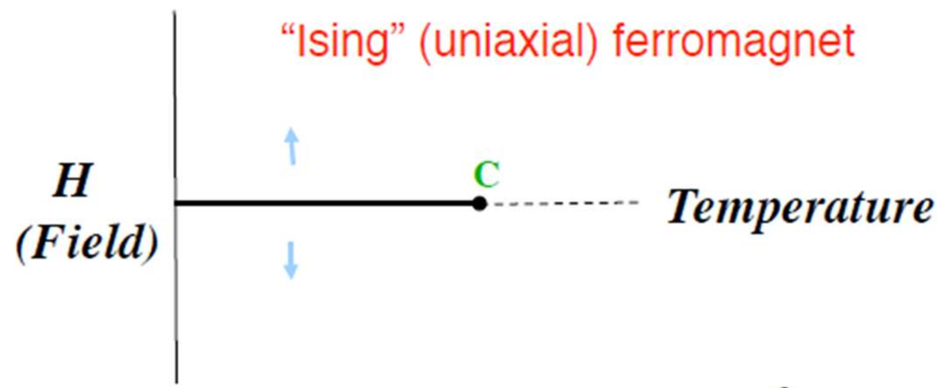
- At high temperature, entropy dominates and leads to a disorder state.
- At low temperature, energy dominates and leads to an ordered state.

→ Landau theory of symmetry-breaking and phase transitions covers this physics in full. It states universality of phase-transitions, and defines an order parameter that spontaneously nucleates below a critical parameter (temperature, field etc.):

<u>Examples:</u>



$$\rho_L - \rho_G \sim \left(\frac{T_C - T}{T_C}\right)^{\beta}$$



$$M_{\uparrow} - M_{\downarrow} \sim \left(\frac{T_C - T}{T_C}\right)^{\beta}$$

$$\text{Experiment}: \quad \beta = 0.322 \pm 0.005$$

$$\text{Theory}: \quad \beta = 0.325 \pm 0.002$$

New order - Topological order

Definition I:

- In a topologically ordered phase, some physical response function is given by a **topological invariant**.

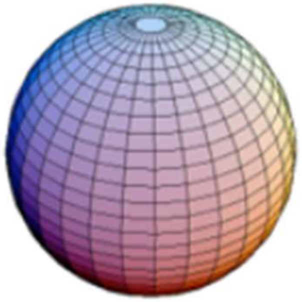
Definition II:

- A topological phase is insulating but always has **metallic edges/surfaces** when put next to a vacuum or an ordinary phase.

Definition III:

- A topological phase is described by a **topological field theory.**

→ Topological invariant is a quantity that does not change under continuous deformation.

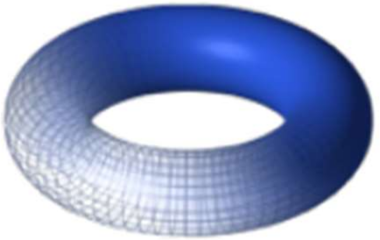


- Most topological invariants in physics arise as integrals of some geometric quantity. At any point of a surface we can define a signed Gaussian curvature:

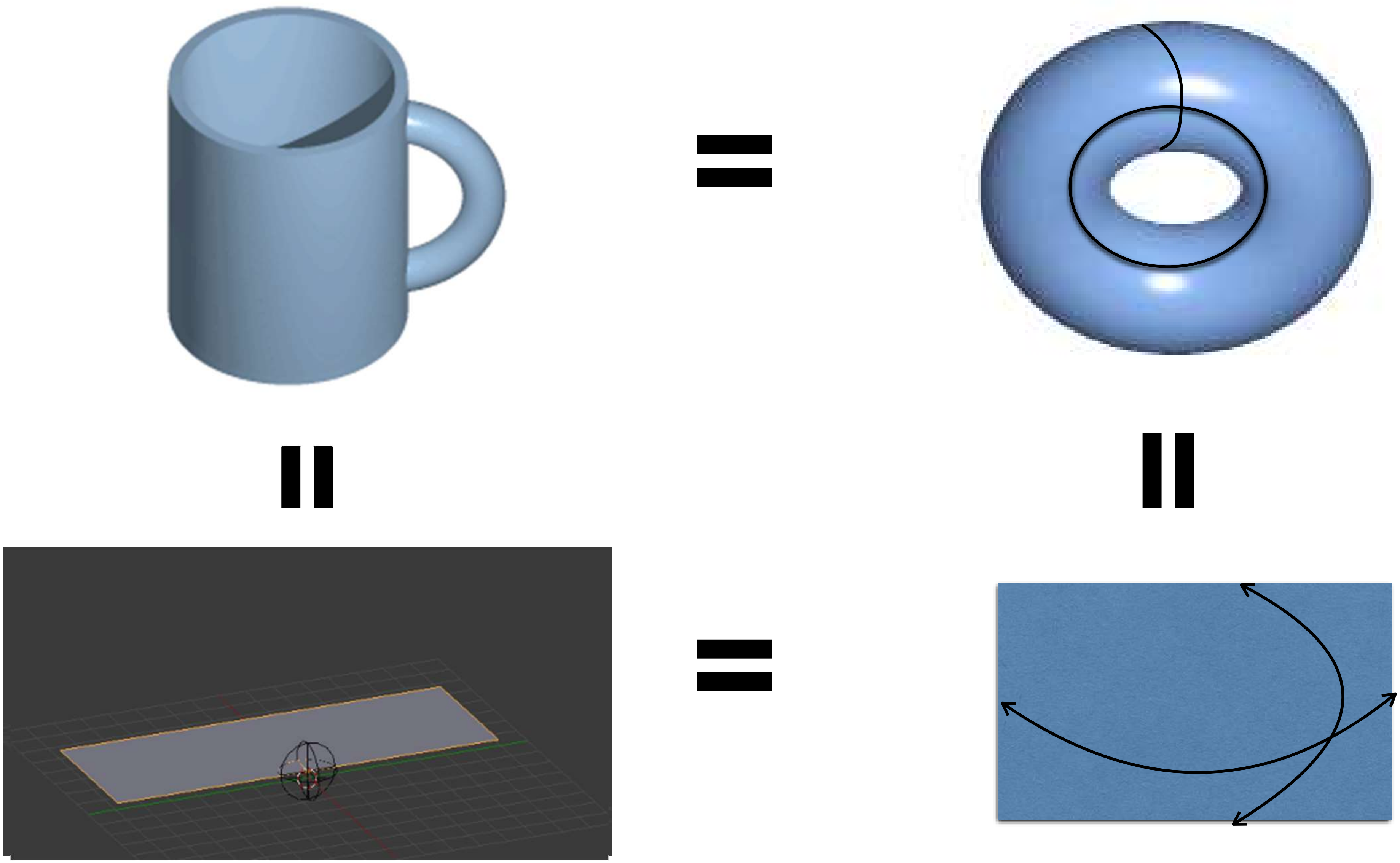
$$\kappa = (r_1 r_2)^{-1}$$

- The area integral of the curvature over the whole surface is quantized, and is a topological invariant (Gauss-Bonnet theorem). Here the genus g = 0 for a sphere, n for n-holed torus etc.

$$\int_M \kappa \, dA = 2\pi\chi = 2\pi(2-2g)$$



Equivalence between shapes in topology

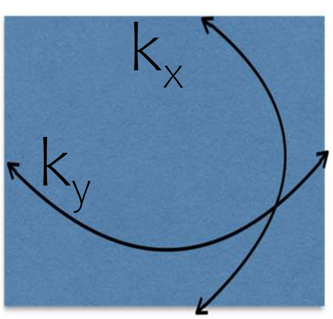


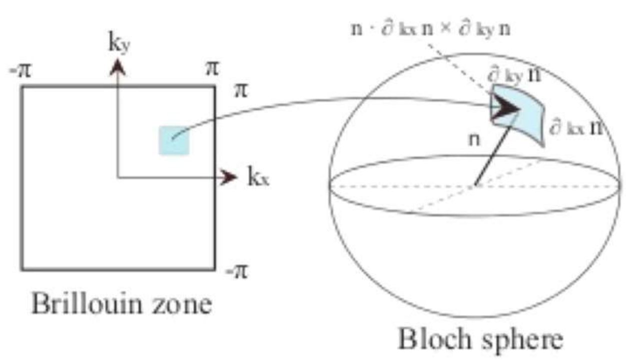
What are the topological invariants in the QHE?

- For the topological invariants in the QHE we need one fact about solids → Blochs theorem.
- The electronic single-particle wavefunctions are maps and hence the classification principles of band dispersions are based on deep notions of topology and quantum geometry.
- One-electron wave-functions in a crystal can be written, where *k* is the crystal momentum and *u* is periodic, with the same periodicity as the unit cell.

$$\psi(\mathbf{r}) = e^{i\mathbf{k}\cdot\mathbf{r}} u_{\mathbf{k}}(\mathbf{r})$$

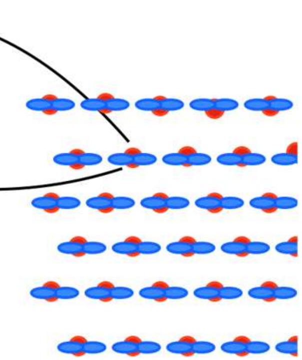
- Crystal momentum *k* can be restricted to the Brillouin zone, a region in k-space with periodic boundaries.
- As *k* changes, we can map out an energy band. Set of all the bands = band structure.
- The Brillouin zone will play the role of the surface as in the previous example.
- And one property of quantum mechanics, the Berry phase will give us the curvature.





$$\psi = (\psi_1, \psi_2) \equiv S^2$$

$$|\psi_1|^2 + |\psi_2|^2 = 1$$



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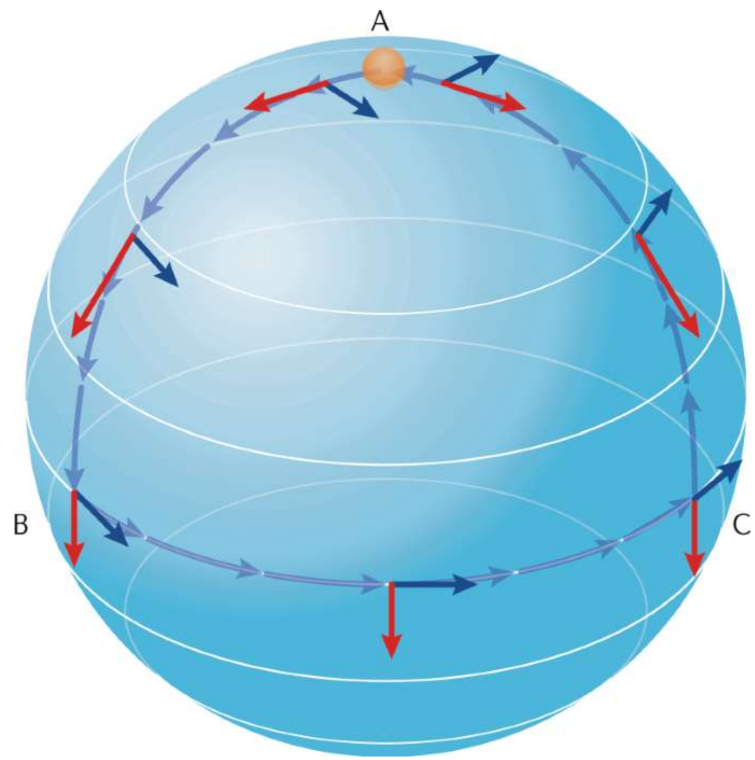
Berry's curvature and phase

- What kind of curvature can exist for electrons in a solid?
- Consider a quantum-mechanical system in its non-degenerate ground-state.
- The adiabatic theorem in quantum mechanics implies that, if the Hamiltonian is changed slowly, the system remains in its time-dependent ground state.
- When the Hamiltonian goes around a closed loop k(t) in parameter space, there can be an irreducible phase relative to the initial phase.



Berry vector potential

$$\mathcal{A} = \langle \psi_k | -i\nabla_k | \psi_k \rangle$$

Berry curvature

$$\Omega(k) = \nabla \times \mathcal{A}$$

Berrys phase

$$\phi = \oint \mathcal{A} \cdot d\mathbf{k}$$

Chern number

$$C = \frac{1}{2\pi} \oint_{BZ} \Omega dk^2 = \nu$$

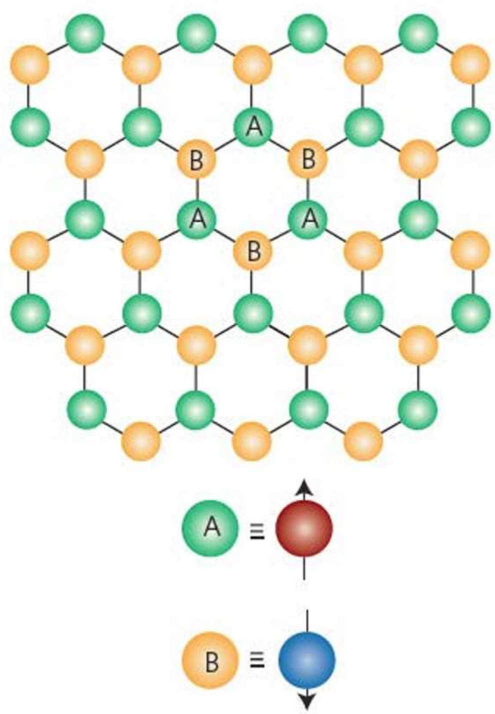
(Plays the role of a fictitious B-field (of orbital nature), vector potential and Aharonov Bohm phase)

Pseudo-spin

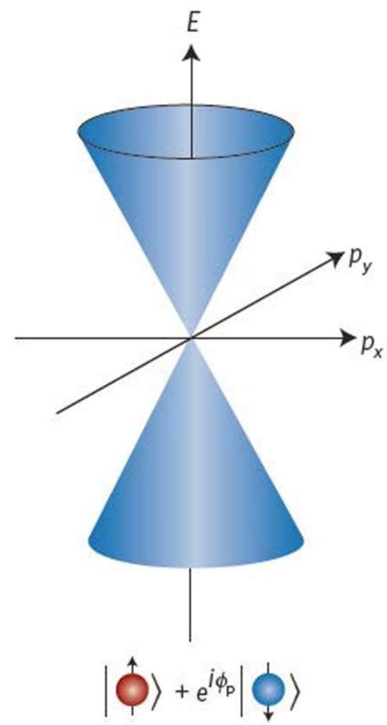
$$\psi_{\vec{k}}(\vec{r}) = \begin{pmatrix}\psi_{\vec{k}A}(\vec{r})\\ \psi_{\vec{k}B}(\vec{r})\end{pmatrix} \sim \frac{1}{\sqrt{2}} e^{i\vec{\kappa}\vec{r}} \begin{pmatrix}1\\ e^{i\theta_\kappa}\end{pmatrix} \to \begin{pmatrix}\psi_\uparrow\\ \psi_\downarrow\end{pmatrix}$$

$$\theta_\kappa = arctan(\kappa_y/\kappa_x)$$

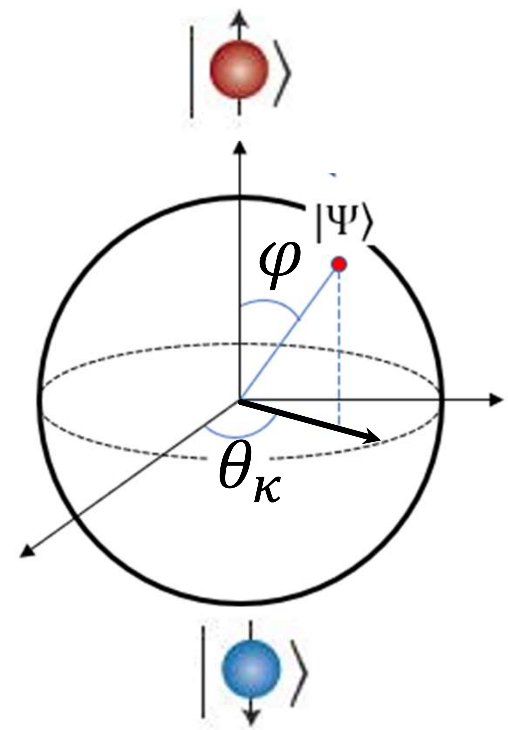
Real space:



Wave functions:



Bloch sphere representation:

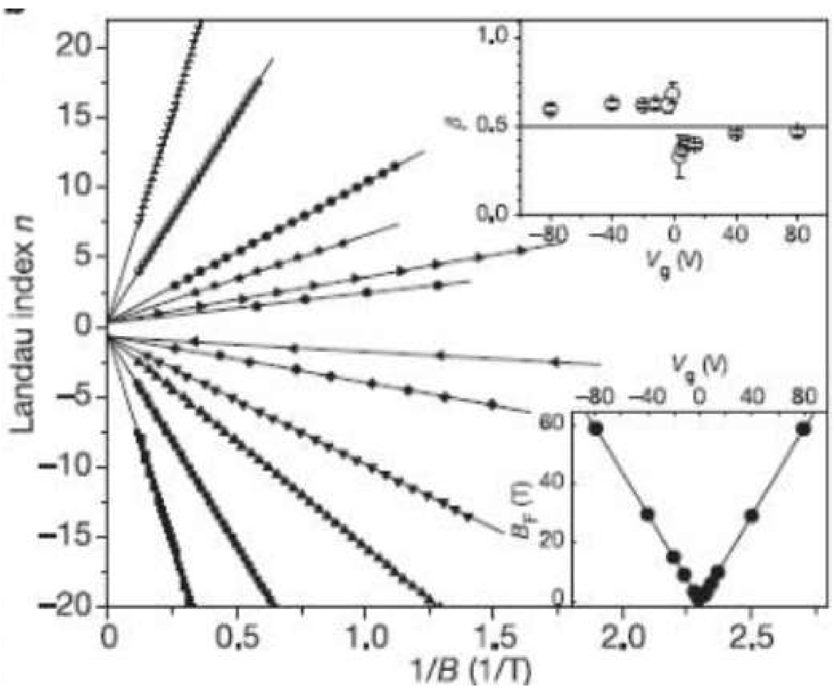


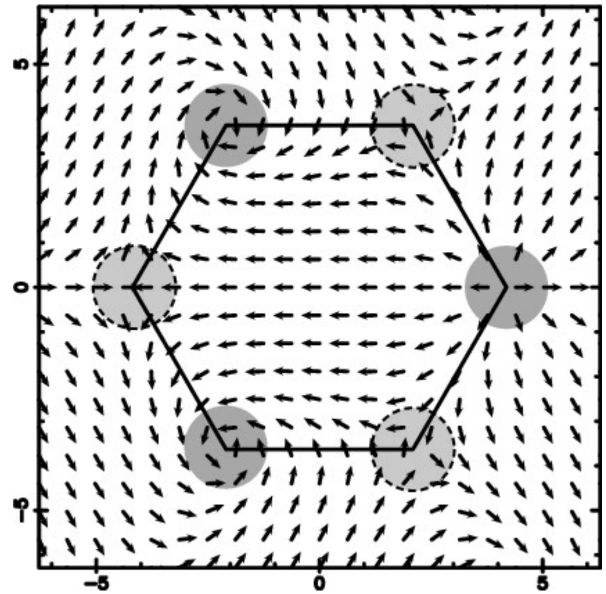
- Pseudo-spin is oriented at the equator → A and B have same amplitudes.

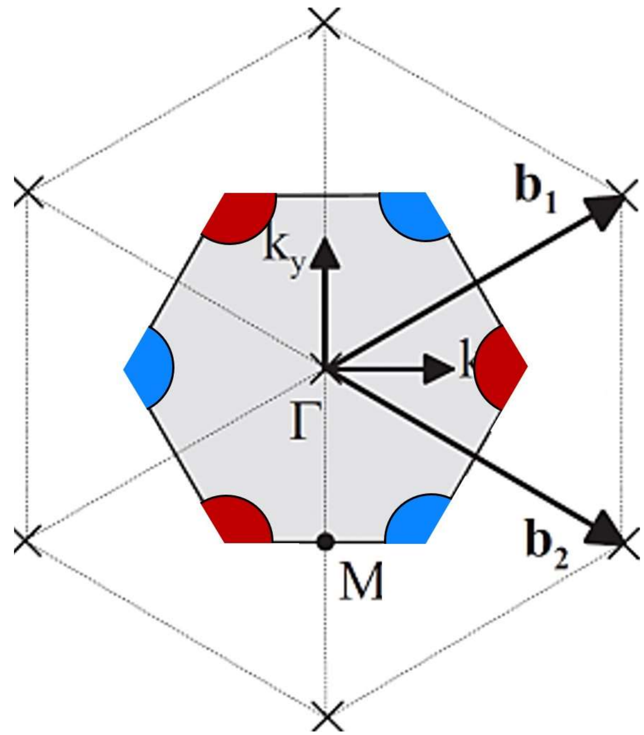
Zero electron mass and Berry curvature in graphene

$$\Delta R_{xx} = R(B,T)\cos[2\pi(B_F/B + 1/2 + \beta)]$$

- B_F = Shubnikov-de Haas Oscillation Frequency in 1/B
- β = Berry Phase
- Aquired when quasiparticle moves between sublattices

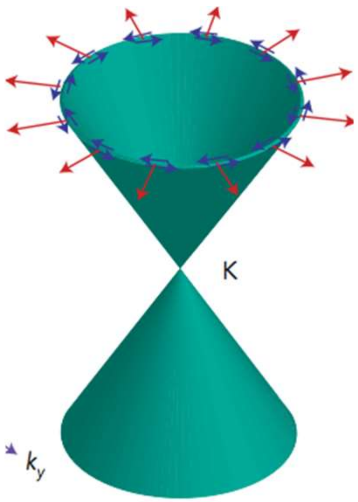


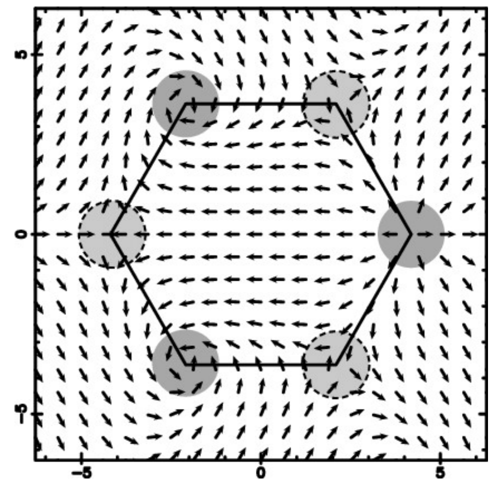


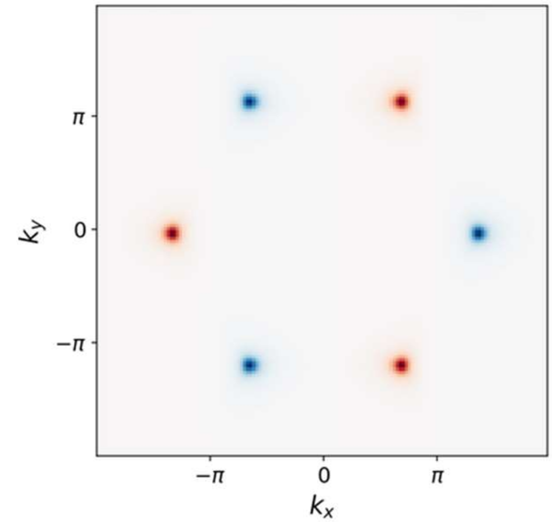


Berry curvature in graphene

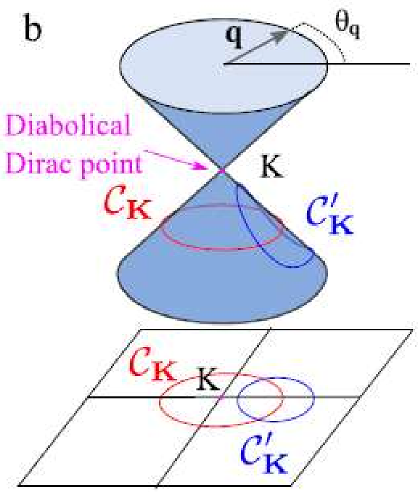
Pseudo-spin textures in k-space:

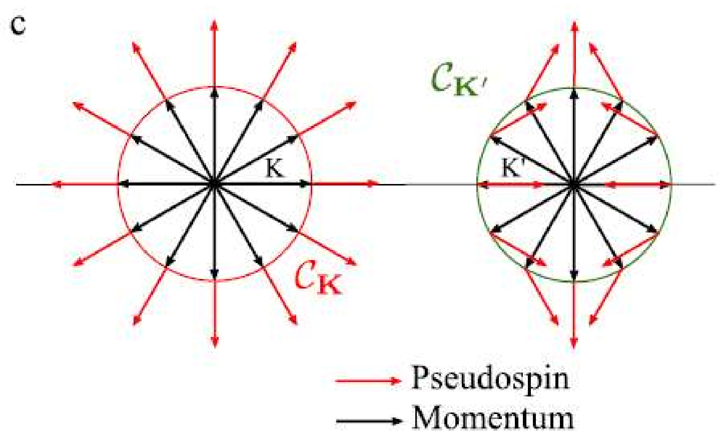






Trajectories around Dirac point in k-space:





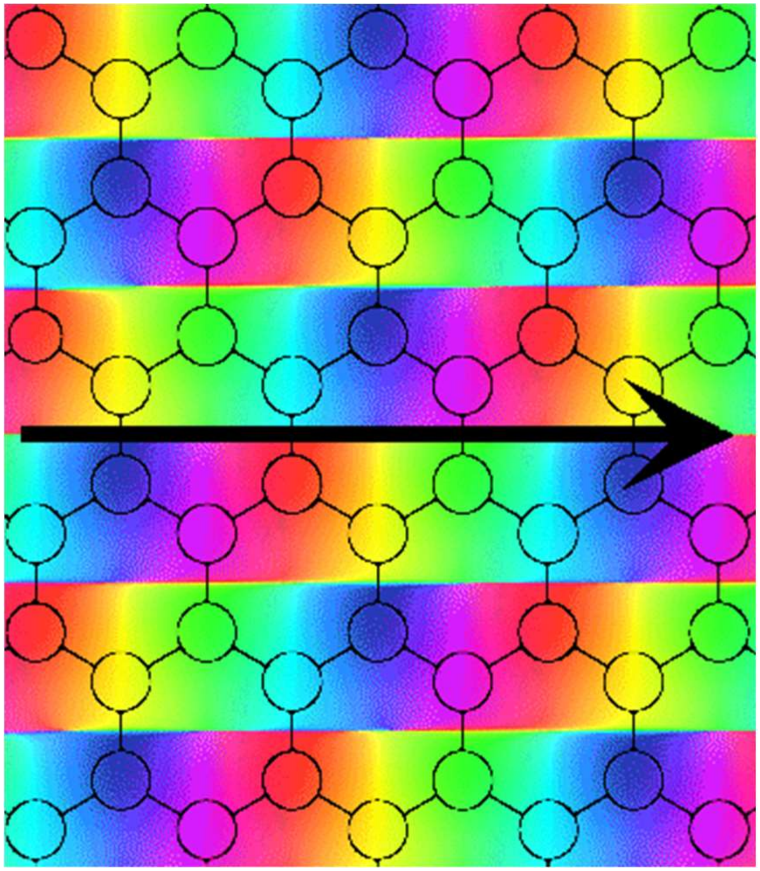
Dirac points are Berry curvature monopoles

$$\Omega(k) = \nabla \times \mathcal{A}$$

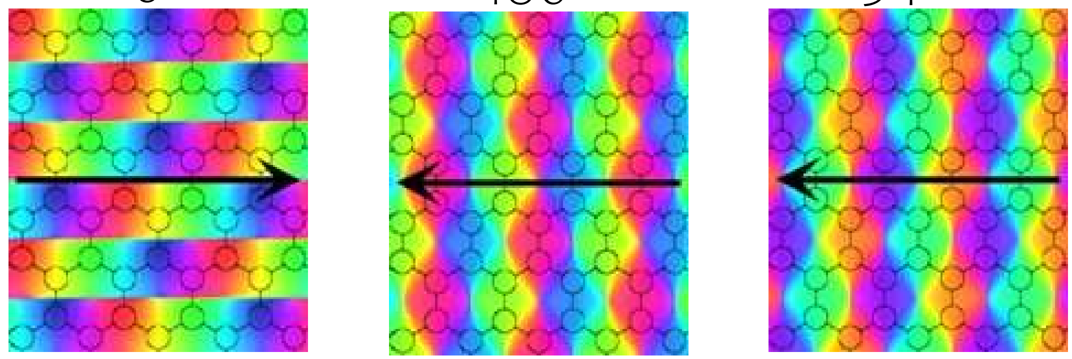
$$C = \frac{1}{2\pi} \oint_{BZ} \Omega \, dk^2 = \nu$$

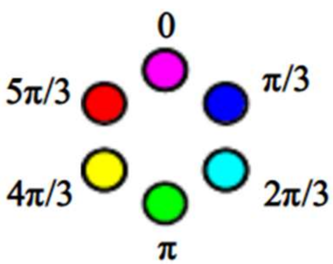
Visualizing pseudo-spin textures

Rotating the k-vector in real space:

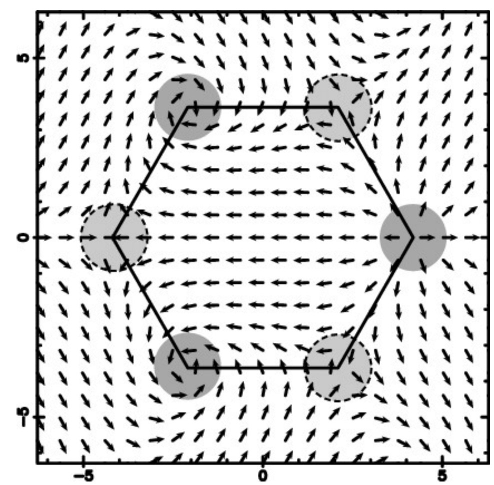


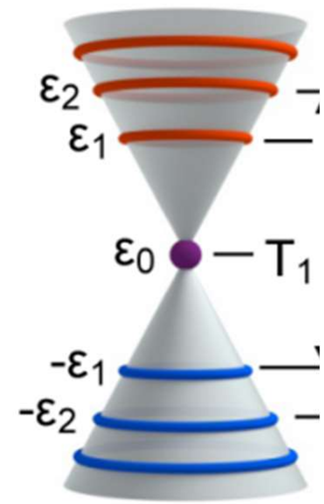
0° 180° 540°





Pseudo-spin textures in k-space:

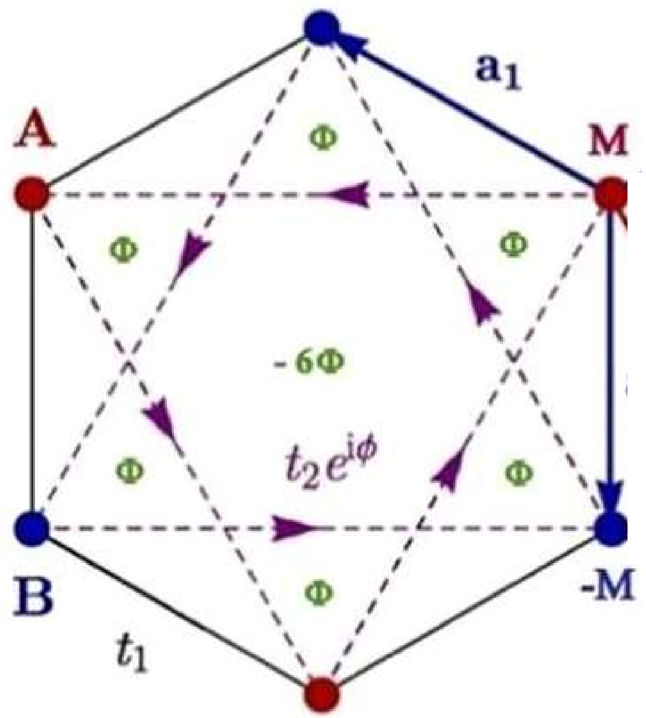




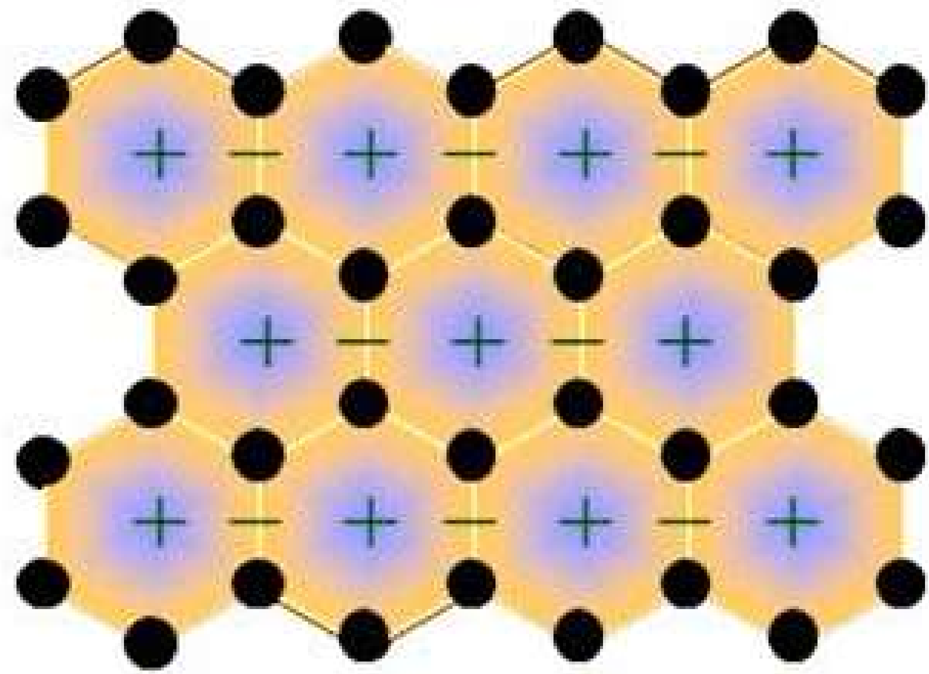
Berry's phase of π and non-trivial topological properties.

Haldane model

Haldane model on a honeycomb lattice:



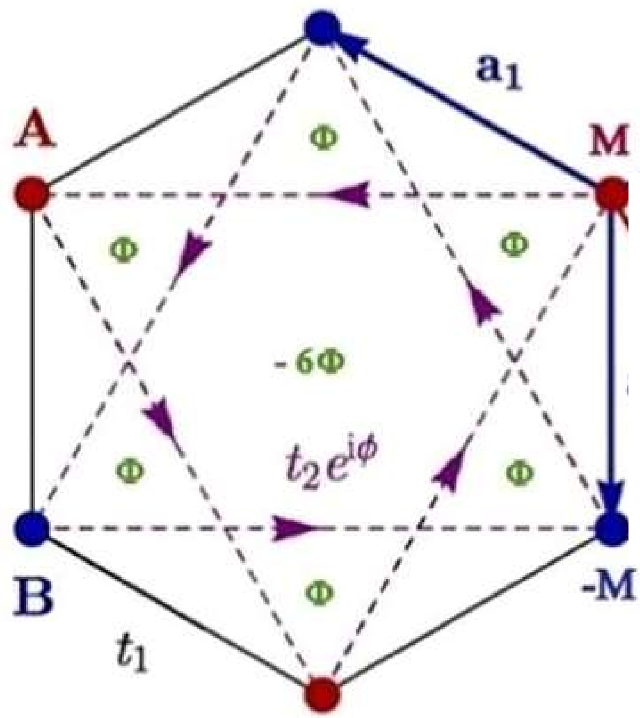
Periodic out of plane B-field:



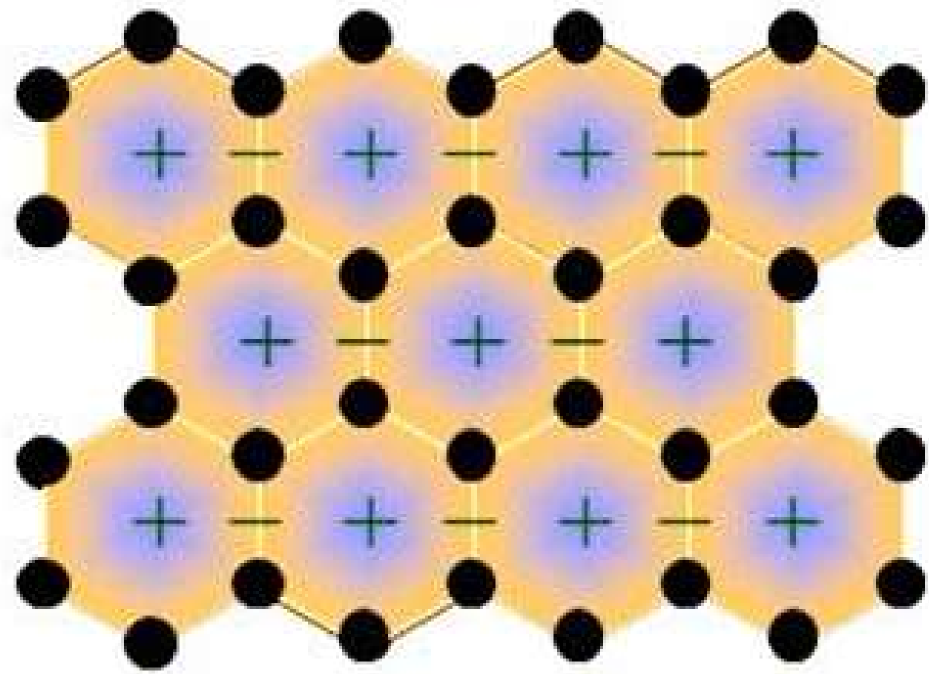
- Graphene has all the key ingredients to be topological, Berry curvature etc.
- How to make graphene topological?
- Haldane model introduces the Haldane mass M (M and –M) on each sub-lattice (A and B), and allows for next nearest neighbor hopping, which is defined by the hopping parameter t_2 and the phase φ.
- This is equivalent to introducing a periodic out of plane magnetic field B.

Haldane model

Haldane model on a honeycomb lattice:



Periodic out of plane B-field:



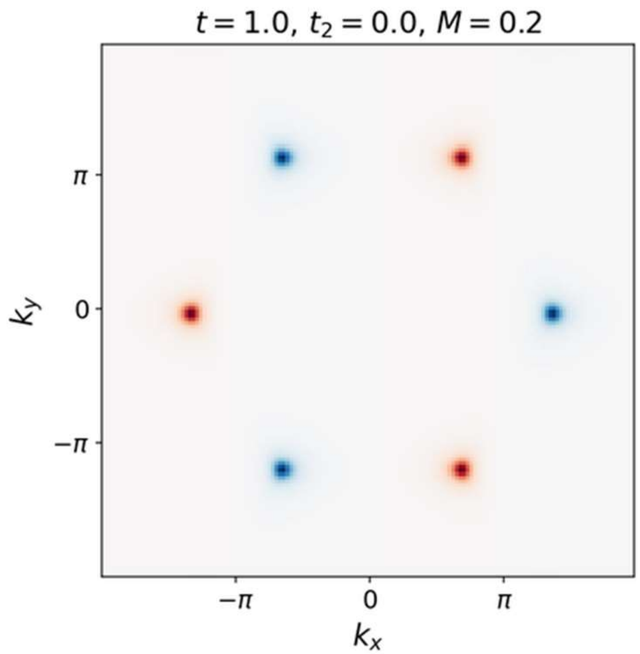
Graphene tight-binding Hamiltonian:

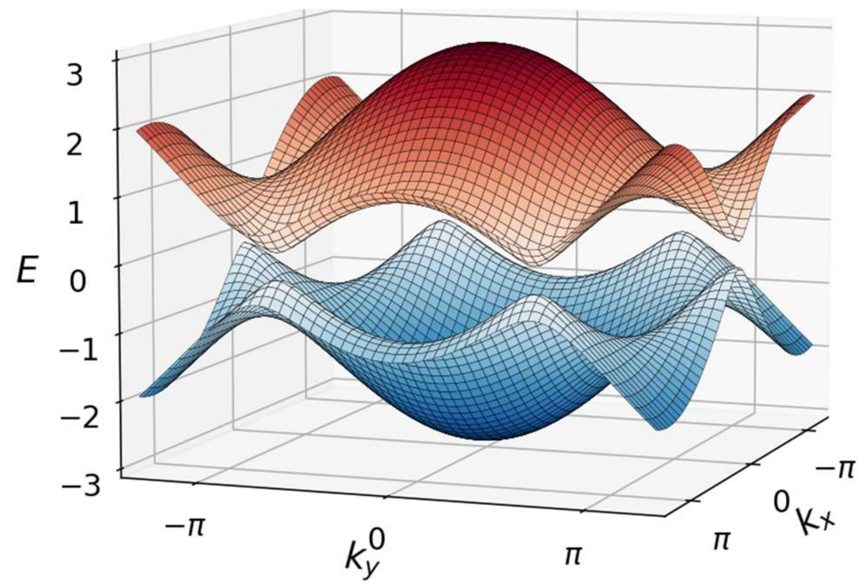
$$H_0(k) := t_1 \cdot \sum_{i=1}^{3} \left(\cos(k \cdot a_i)\sigma_x - \sigma_y \sin(k \cdot a_i) \right)$$

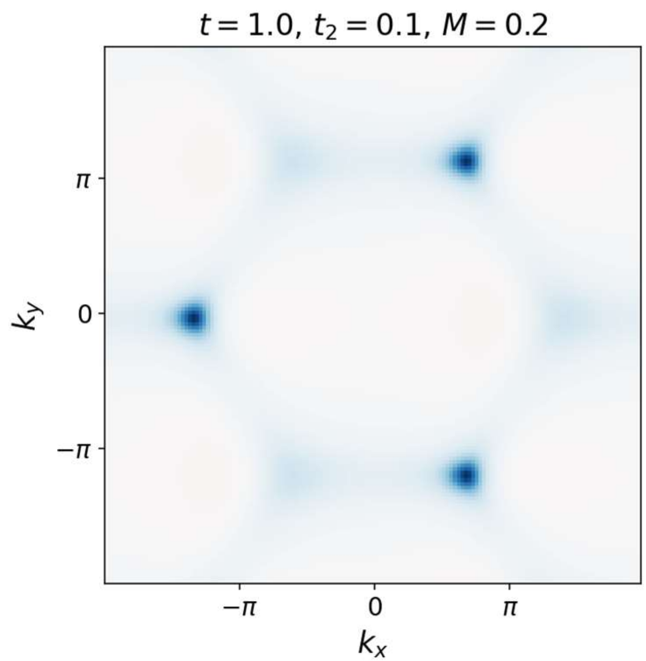
Haldane model:

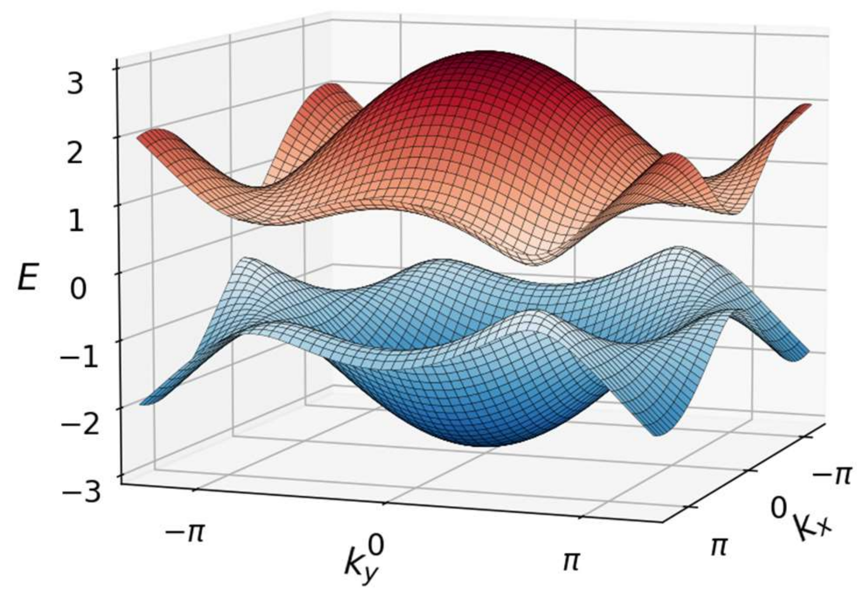
$$H(k) := H_0(k) + \underbrace{\left(M + 2t_2 \sum_{j=1}^{3} \sin(k \cdot b_i) \right) \cdot \sigma_z}_{\text{massterm}}$$

Haldane model – Berry curvature

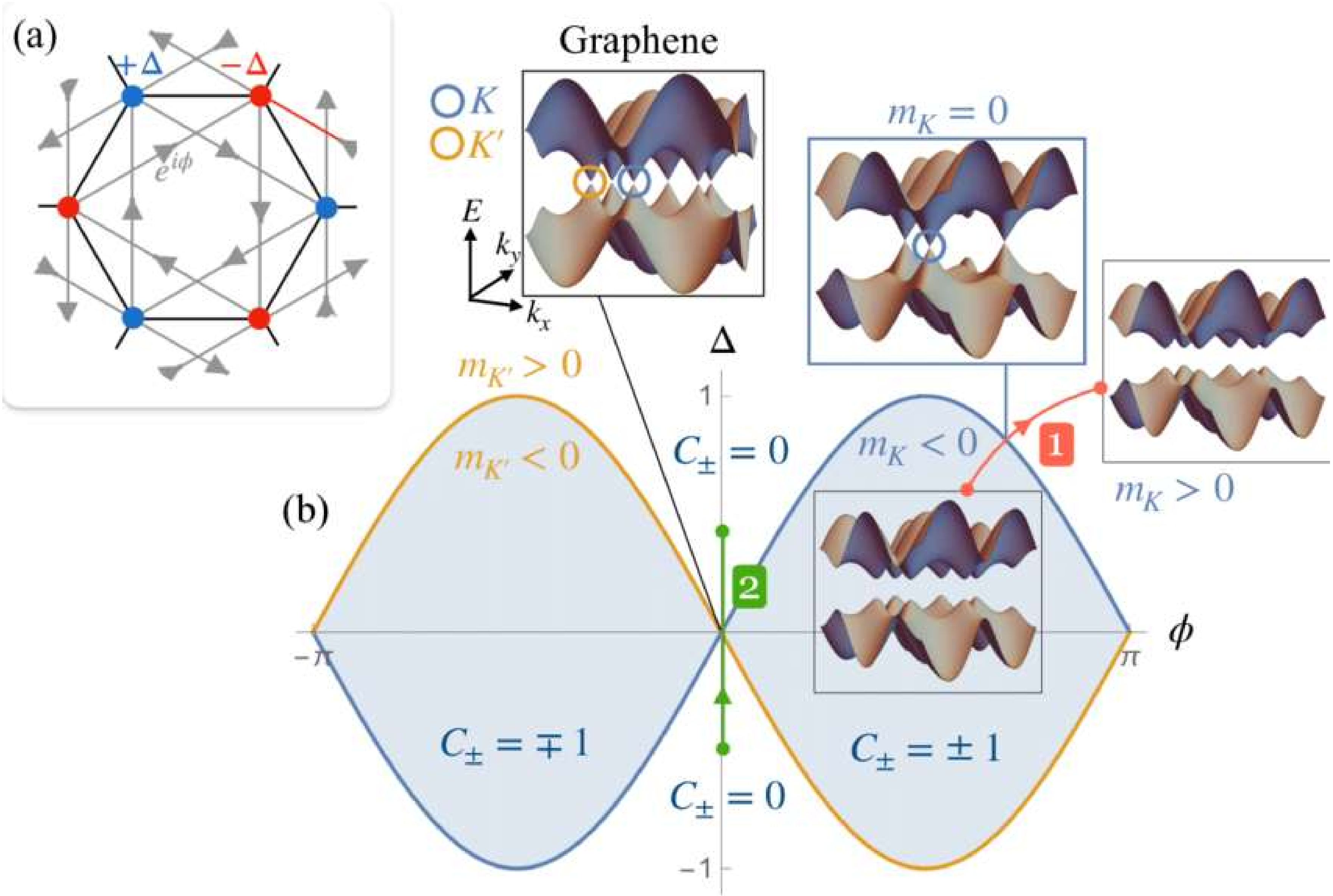






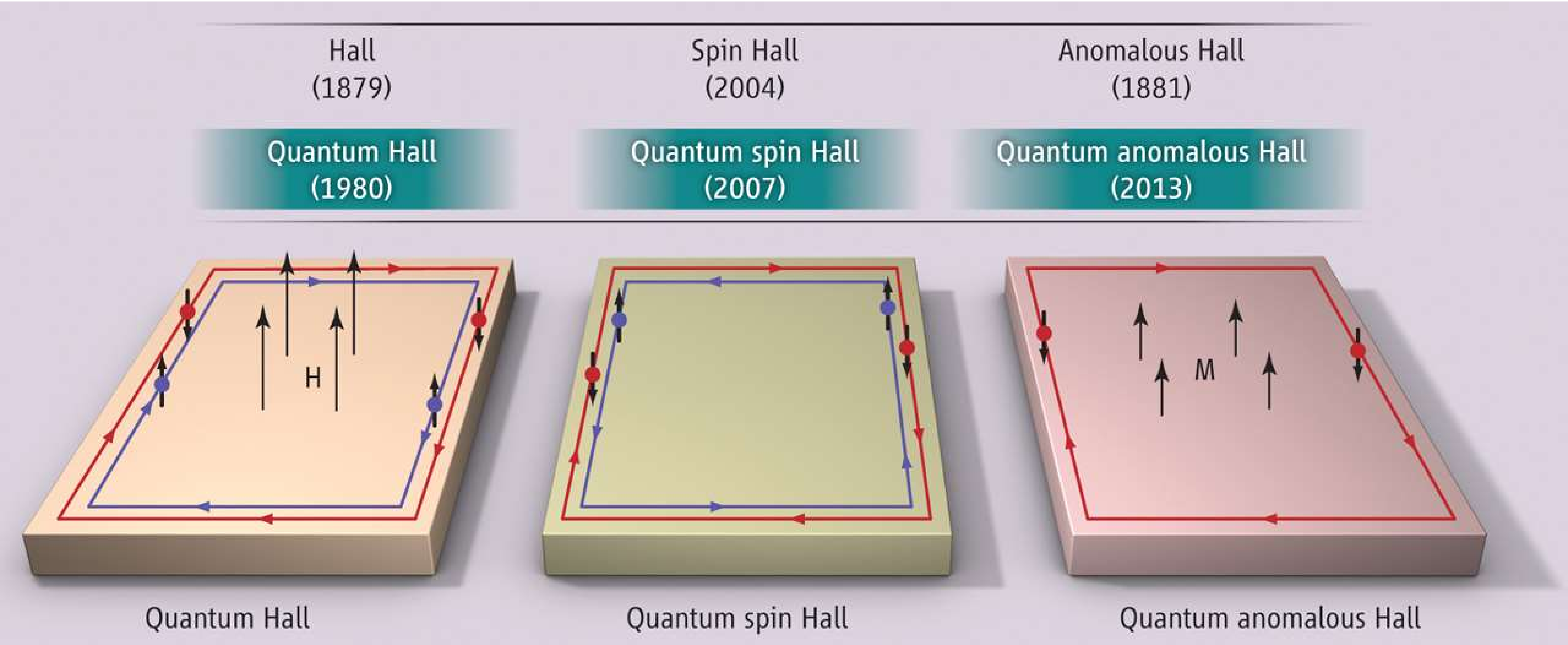


Haldane model – Chern numbers



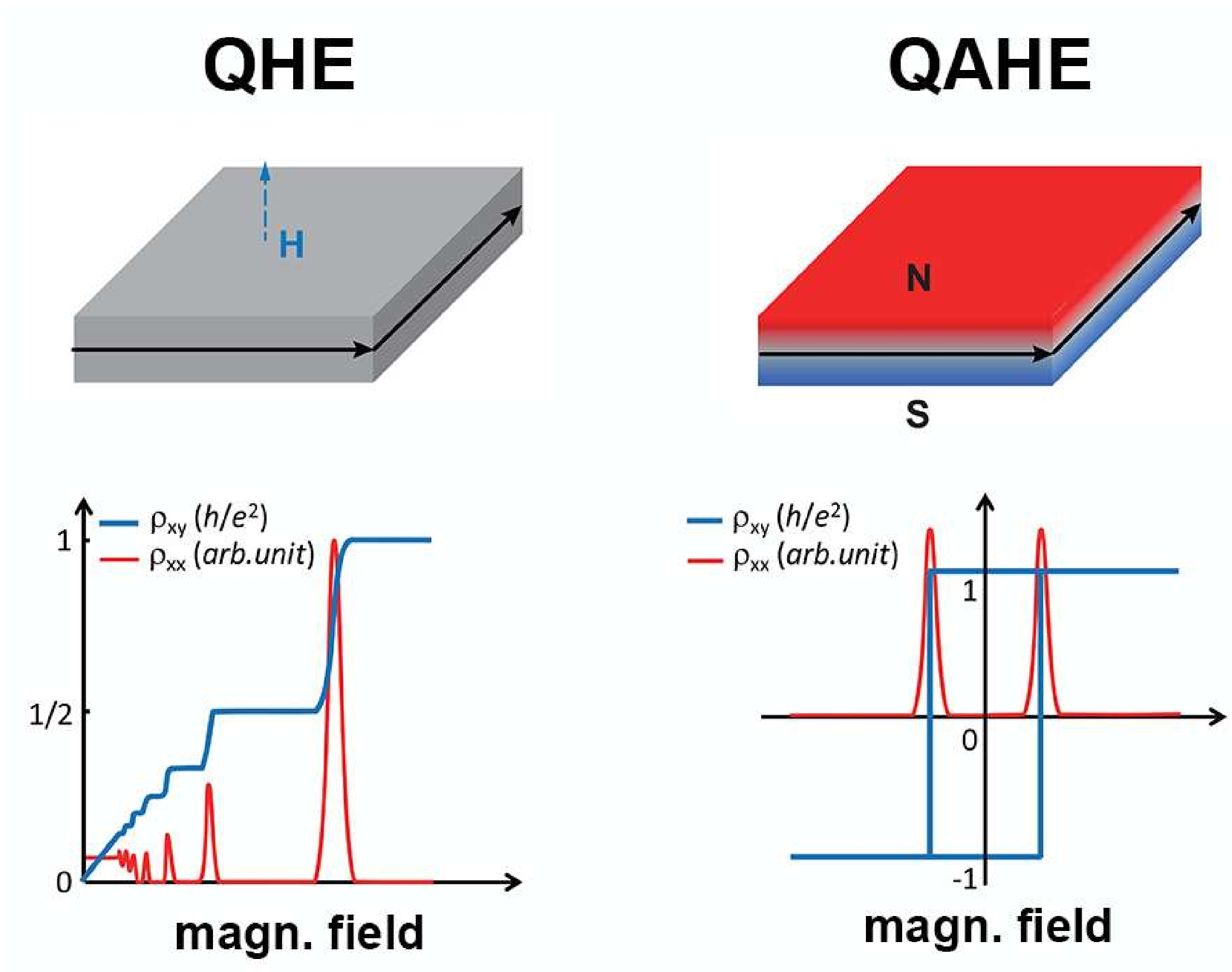
- Integration of the Berry curvature over BZ gives rise to topological Chern bands, with Chern number 1 and -1.

Quantum Hall Effect without B-field



- Quantum Spin Hall effect and Quantum Anomalous Hall effect – Quantum Hall effect in zero magnetic field, given rise by a combination of topological electron states and a strong spin-orbit coupling and/or ferromagnetic bulk of the material.

Quantum Hall without B-field (LLs)



- Quantum Anomalous Hall effect – even in zero B-field the bulk is insulating and edge states develop R_{xx} = 0 and R_{xy} = (h/e^2)
- Reversing of the B-field flips the magnetization direction and the direction of the edge state.

2D Topological insulators

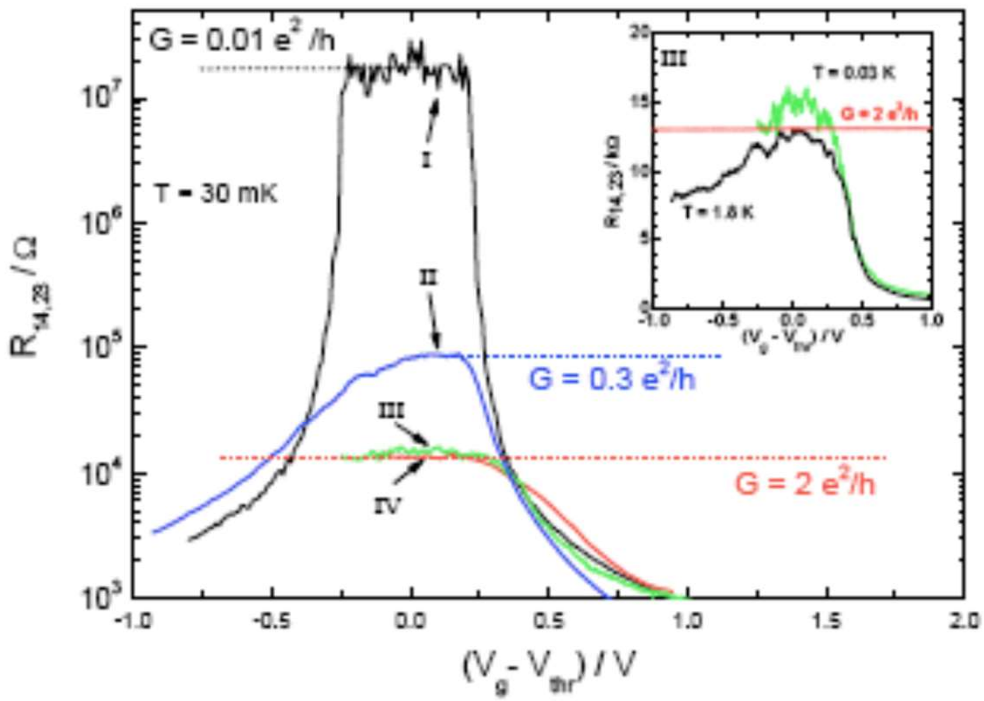
Key: the topological invariant predicts the "number of quantum wires".

While the wires are not one-way, so the Hall conductance is zero, they still contribute to the *ordinary* (two-terminal) conductance.

There should be a low-temperature *edge* conductance from one spin channel at each edge:

$$G = \frac{2e^2}{h}$$

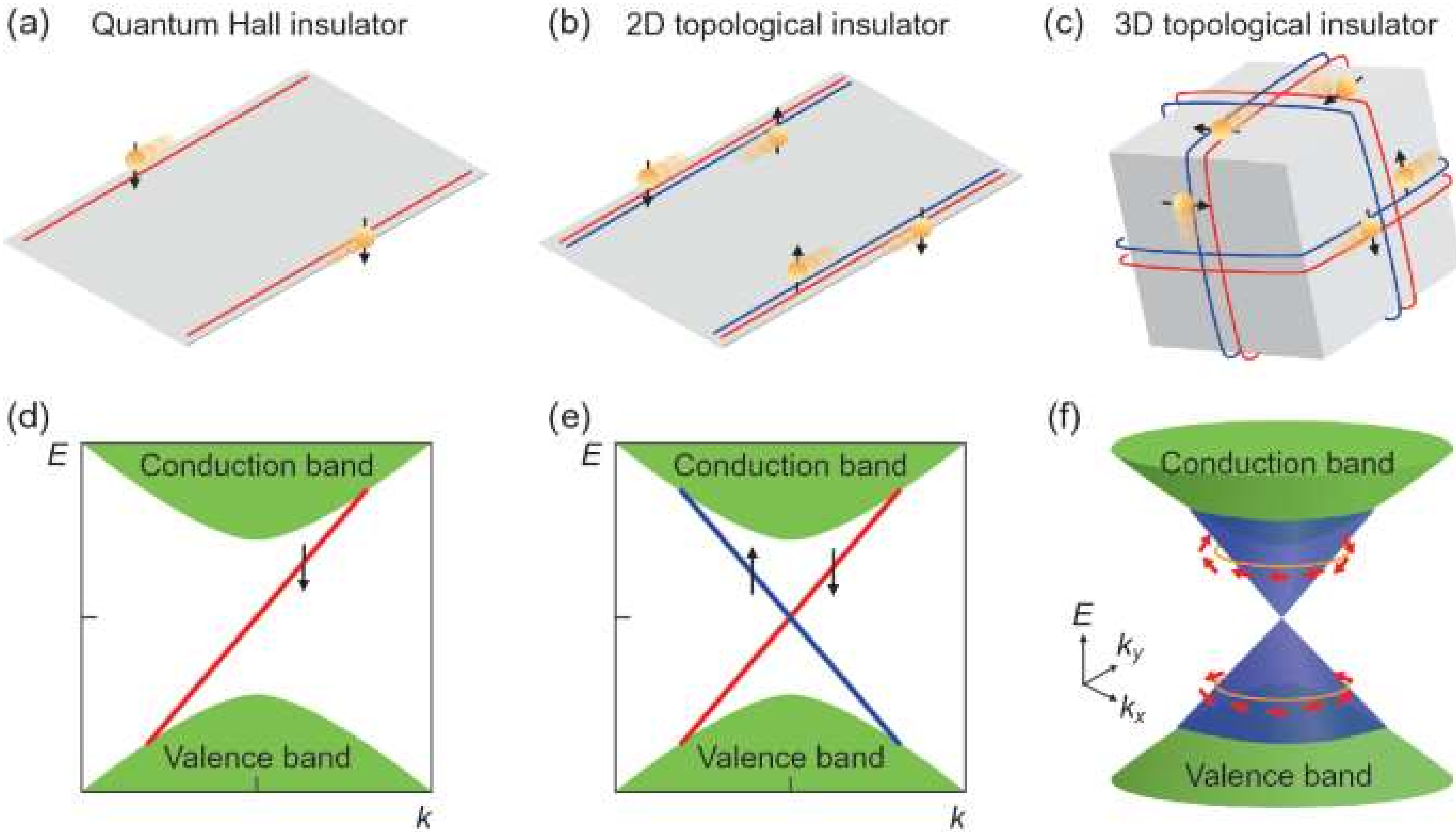
König et al., *Science* (2007)



Laurens Molenkamp

This appears in (Hg,Cd)Te quantum wells as a quantum Hall-like plateau *in zero magnetic field.*

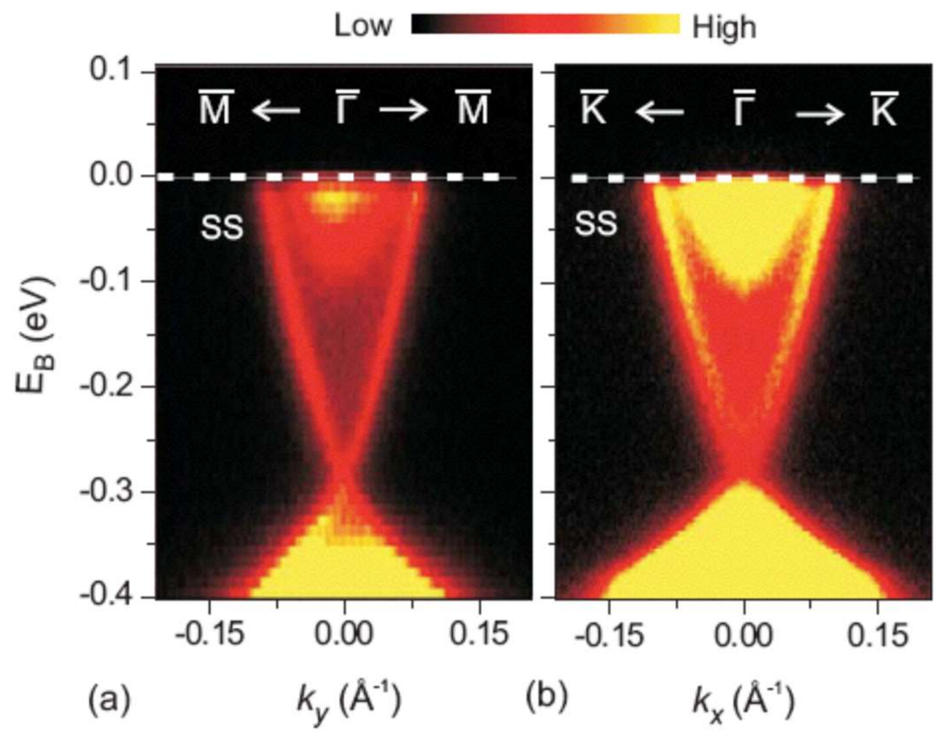
3D Topological insulators



3D Topological insulators

First observation by D. Hsieh et al. (Z. Hasan group), Princeton/LBL, 2008.

This is later data on Bi_2Se_3 from the same group in 2009:



The states shown are in the "energy gap" of the bulk material--in general no states would be expected, and especially not the Dirac-conical shape.