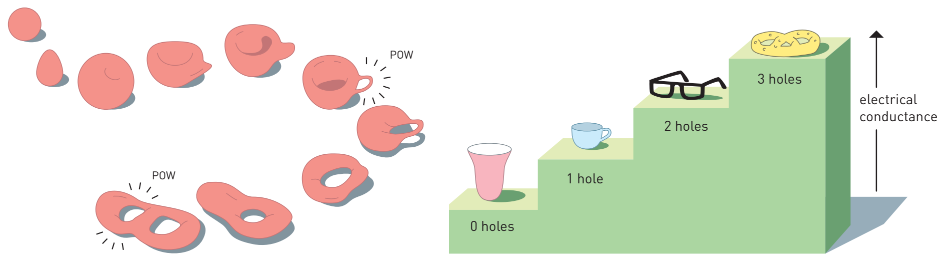

Topology in nonrelativistic quantum mechanic

Raffaele Resta

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La Sapienza, Roma, January 24th, 2017

Outline

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Archetypes

1954 Yang-Mills gauge theory (relativistic QM)

Geometrical meaning understood only in the **1970s**, after C.N. Yang interacted with mathematicians (Singer, Atiyah, Chern...)

1959 Aharonov-Bohm experiment (nonrelativistic QM)

Geometrical meaning understood only after the famous paper by Michael Berry (**1984**)

1982 From geometry to topology: **TKNN**
(**T**houless, **K**ohmoto, **N**ightingale, and den **N**ijs)

Aharonov-Bohm, 1959

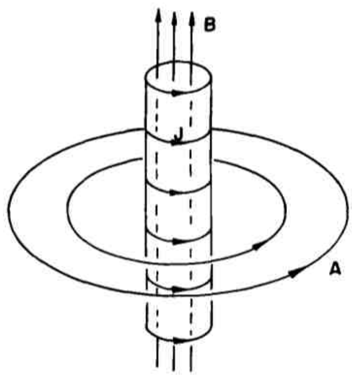
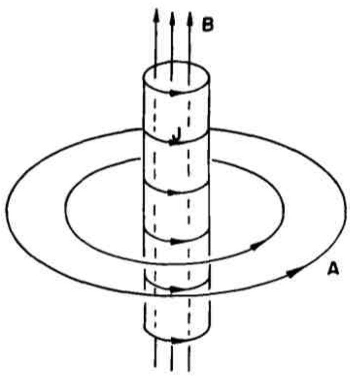


Fig. 15–6. The magnetic field and vector potential of a long solenoid.

- Figure from Feynman, Vol. 2 (1963)
- Main message:
  - Classical particles: only the **fields** may act on them
  - Quantum particles: the **potentials** act on them even when no field is present
  - **Why** such difference?

Aharonov-Bohm, 1959



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Berry phase, 1984

- Very simple concept, nonetheless missed by the founding fathers of QM in the 1920s and 1940s
- Nowadays in any modern elementary QM textbook

- After Berry, we have two kinds of **observables**:
  - Expectation values of some **operator**
  - Gauge-invariant **phases** of the wavefunction (no operator whatsoever)

- **Main message:**
  In QM anything gauge-invariant is in principle observable!

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Michael Berry

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Topology

- Branch of mathematics that describes properties which remain unchanged under smooth deformations
- Such properties are often labeled by integer numbers: **topological invariants**
- Founding concepts: continuity and connectivity, open & closed sets, neighborhood......
- Differentiability or even a metric **not** needed (although most welcome!)

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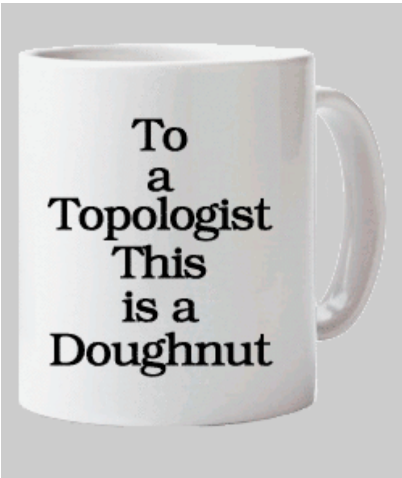
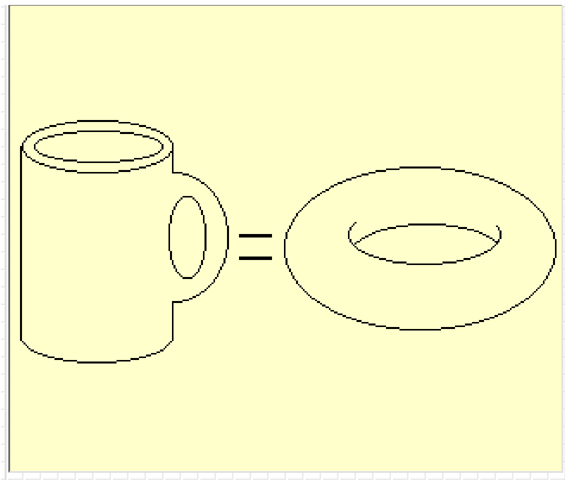
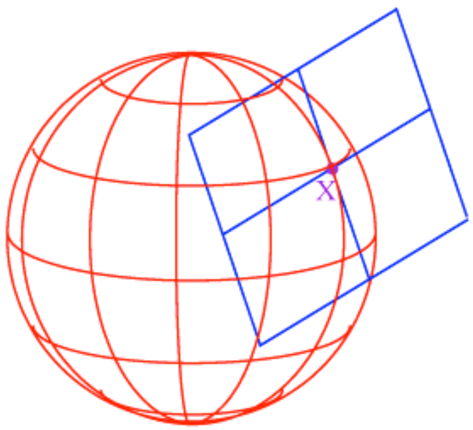
A coffee cup and a doughnut are the same





Topological invariant: **genus** (=1 here)

Gaussian curvature: sphere



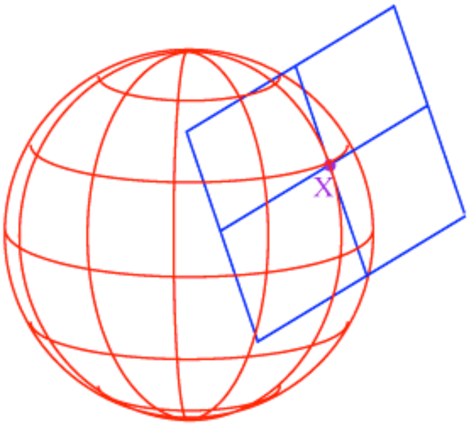
In a local set of coordinates in the tangent plane

$$z = R - \sqrt{R^2 - x^2 - y^2} \simeq \frac{x^2 + y^2}{2R}$$

Hessian $$H = \begin{pmatrix} 1/R & 0 \\ 0 & 1/R \end{pmatrix}$$

Gaussian curvature $$K = \det H = \frac{1}{R^2}$$

Gaussian curvature: sphere



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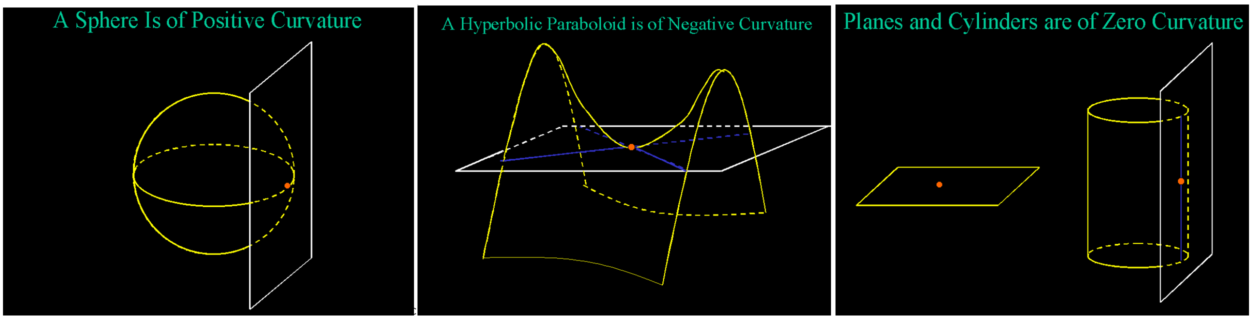
Positive and negative curvature

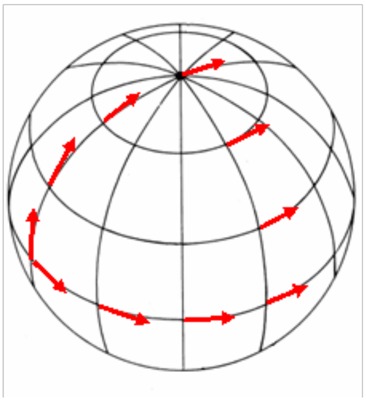


Smooth surface, local set of coordinates on the tangent plane

$$K = \det \begin{pmatrix} \frac{\partial^2 z}{\partial x^2} & \frac{\partial^2 z}{\partial x \partial y} \\ \frac{\partial^2 z}{\partial y \partial x} & \frac{\partial^2 z}{\partial y^2} \end{pmatrix}$$

Twist angle vs. Gaussian curvature

Gaussian curvature of the spherical surface $K = 1/R^2$



- Angular mismatch for parallel transport:

$$\gamma = \int d\sigma \; K$$

- Equivalently: sum of the three angles:

$$\alpha_1 + \alpha_2 + \alpha_3 = \pi + \gamma = \pi + \int d\sigma \; K$$

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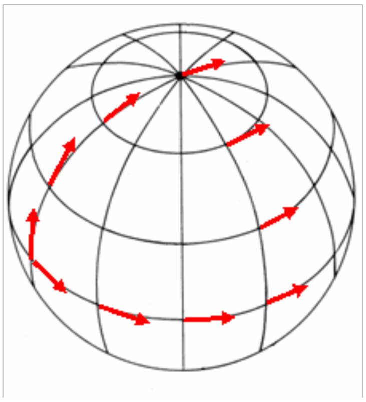

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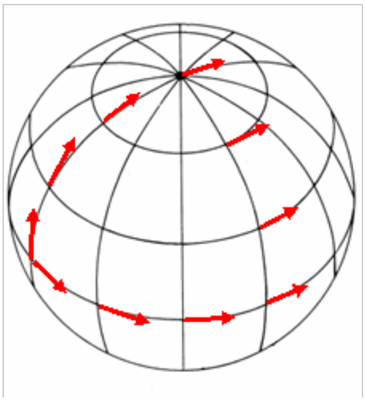
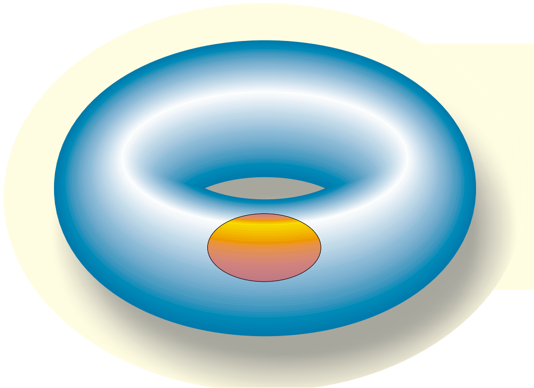
What about integrating over a closed surface?





- Sphere:

$$K = \frac{1}{R^2}, \qquad \int d\sigma\ K = 4\pi R^2 \frac{1}{R^2} = 4\pi$$

- Torus:

$$\int d\sigma\ K = \quad ???$$

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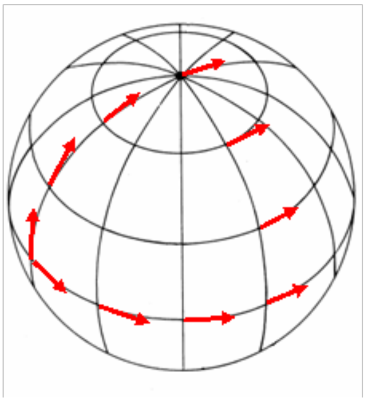
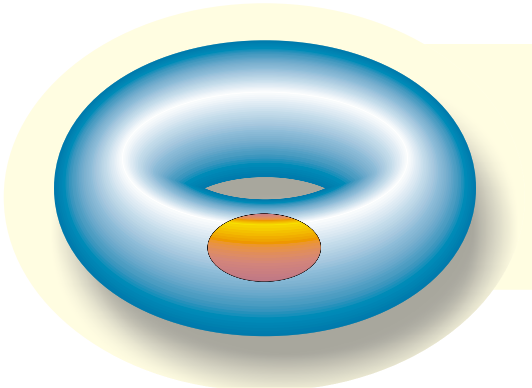

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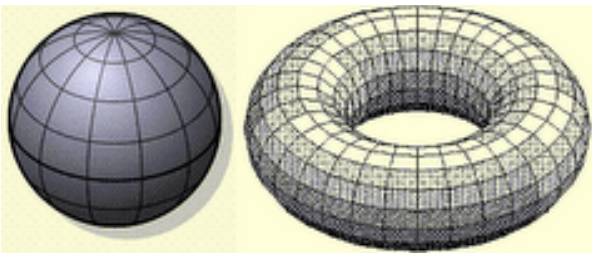
Gauss-Bonnet theorem (1848)

Over a smooth closed surface:

$$\frac{1}{2\pi}\int_S d\sigma\; K = 2(1-g)$$

- Genus g integer: counts the number of "handles"
- Same g for homeomorphic surfaces
  (continuous stretching and bending into a new shape)
- Differentiability not needed



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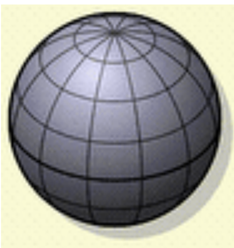

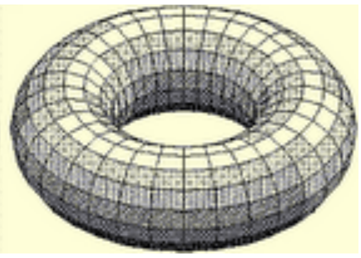

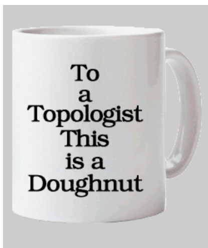

$g = 0$ $\qquad g = 1$ $\qquad g = 1$ $\qquad g = 2$

Outline

Integer quantum Hall effect

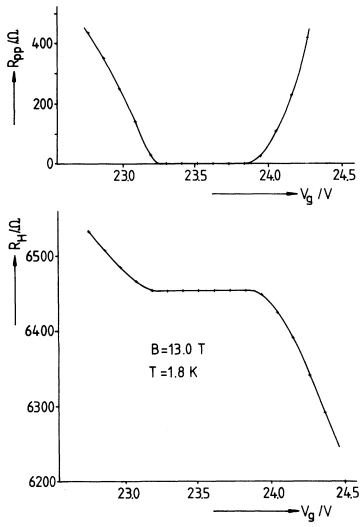

Figure from von Klitzing et al. (1980).

Gate voltage V_g was supposed to control the carrier density.

Plateau flat to five decimal figures

Natural resistance unit:
1 klitzing $= h/e^2 = 25812.807557(18)$ ohm.
This experiment: R_{H} = klitzing / 4

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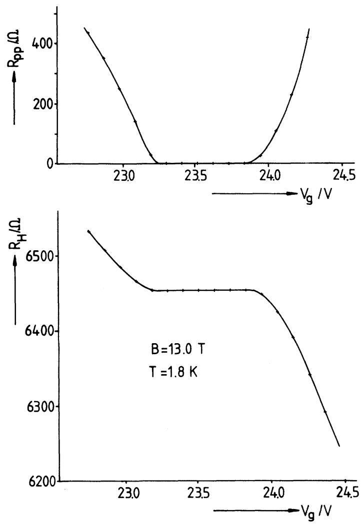

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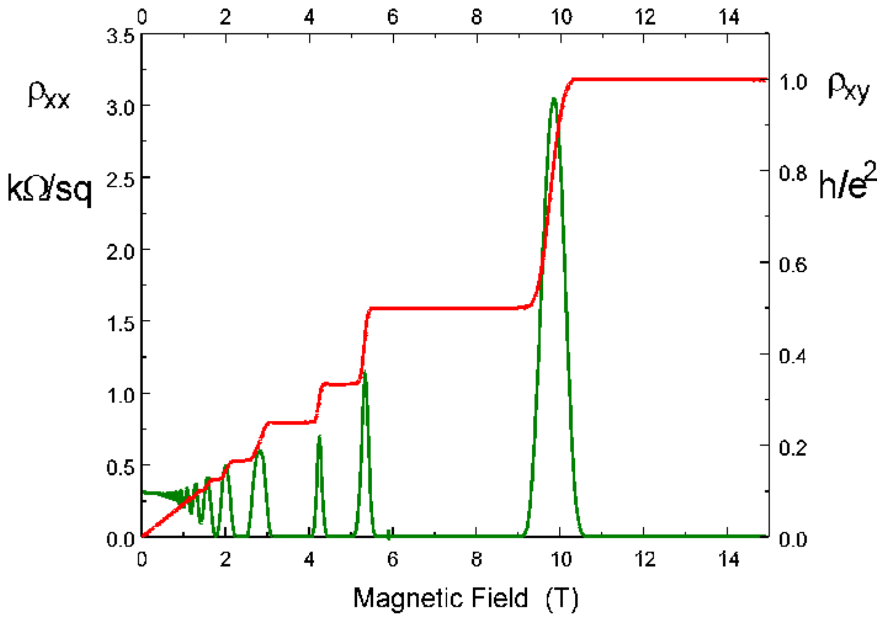
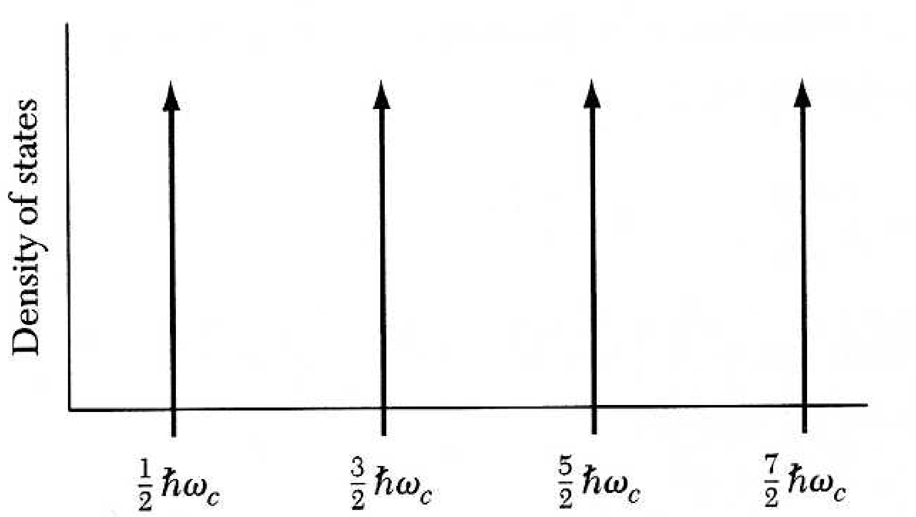
More recent experiments



GaAs-GaAlAs heterojunction, at 30mK

- Plateaus accurate to nine decimal figures
- In the plateau regions $\rho_{xx} = 0$ **and** $\sigma_{xx} = 0$: "quantum Hall insulator"

Landau levels (flat potential)

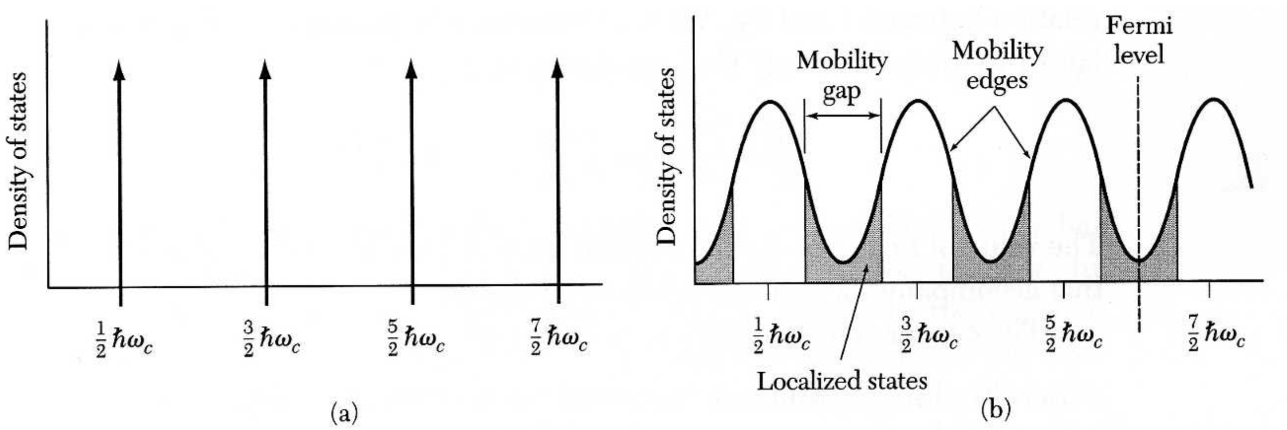


- Number of states in each Landau level: $\frac{B \times \text{area}}{hc/e}$
- $\sigma_{xx} = 0$ seems to require **very** fine tuning!

Continuous “deformation” of the wave function

- Topological invariant:
  Quantity that does not change under continuous deformation

- From a **clean** sample (flat substrate potential)
  to a **dirty** sample (disordered substrate potential)
- σ_{xy} is some **“genus”** of the ground-state wavefunction



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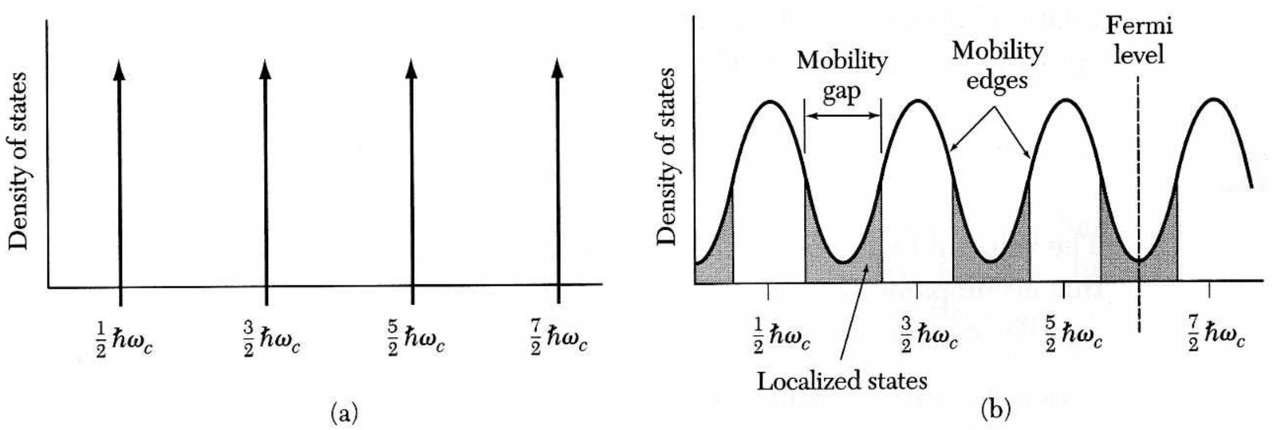

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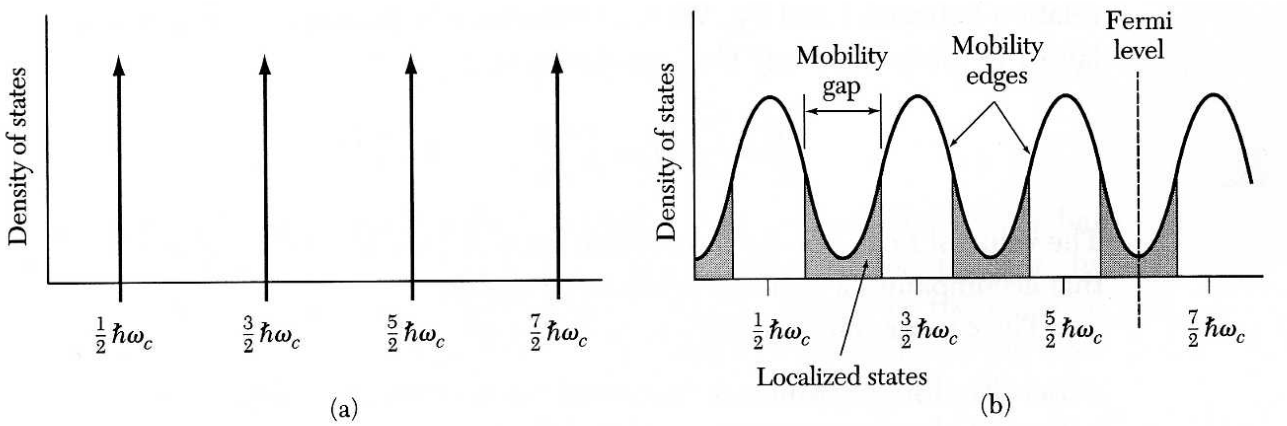
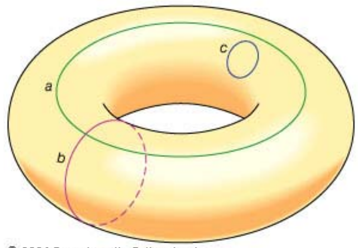


Outline

Quantum Mechanics: Berry curvature

Parametric Hamiltonian
on a closed surface (a torus) :
$H(\vartheta, \varphi) = H(\vartheta + 2\pi, \varphi) = H(\vartheta, \varphi + 2\pi)$

Ground **nondegenerate** eigenstate $|\psi_0(\vartheta, \varphi)\rangle$



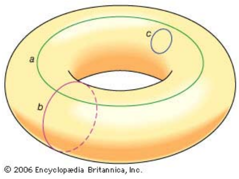
- Berry curvature:

$$\Omega(\vartheta, \varphi) = i \left(\langle \frac{\partial}{\partial \vartheta} \psi_0 | \frac{\partial}{\partial \varphi} \psi_0 \rangle - \langle \frac{\partial}{\partial \varphi} \psi_0 | \frac{\partial}{\partial \vartheta} \psi_0 \rangle \right)$$

- Chern theorem (1944):

$$\frac{1}{2\pi} \int_0^{2\pi} d\vartheta \int_0^{2\pi} d\varphi \;\; \Omega(\vartheta, \varphi) = C_1 \;\in \mathbb{Z}$$

Compare Gauss-Bonnet with Chern



- Gauss-Bonnet theorem:

$$\frac{1}{2\pi}\int_S d\sigma\, K = 2(1-g), \quad g = 0, 1, 2, \ldots$$

- Gauss-Bonnet-Chern theorem:

$$\frac{1}{2\pi}\int_S d\sigma\, \Omega = C_1, \quad C_1 \in \mathbb{Z}$$

- Very robust under deformations of $H(\vartheta, \varphi)$:
  C_1 stays constant insofar as the ground state stays **nondegenerate**

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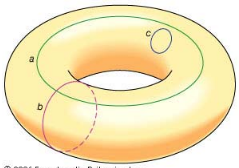

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Back to the IQHE

TKNN:

- Start from the standard **Kubo formula** for conductivity σ_{xy}
- Then transform into $\sigma_{xy} = \frac{h}{e^2} C_1 = C_1 \; klitzing^{-1}$

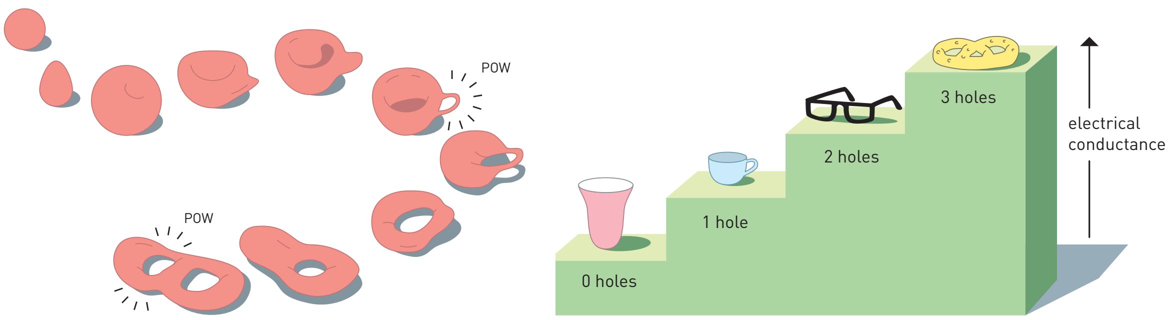
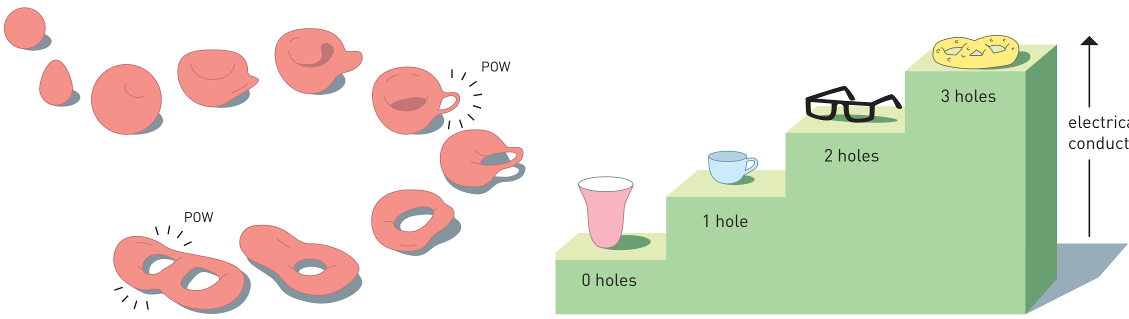
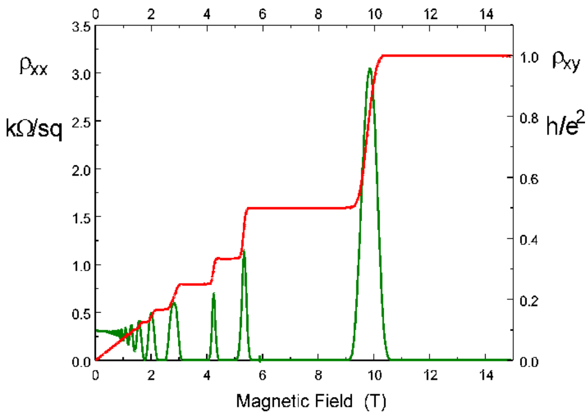


Figure downloaded from http://www.nobelprize.org

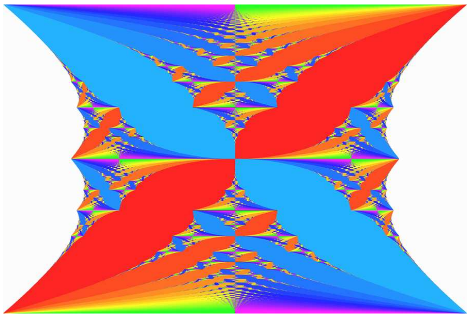
Robust insofar as the system remains **insulating**





Weirdness of macroscopic **B** fields

- The Hamiltonian **cannot** be lattice periodical
- Besides IQHE, other weird phenomena were known
- For instance, the Hofstadter butterfly (1976):



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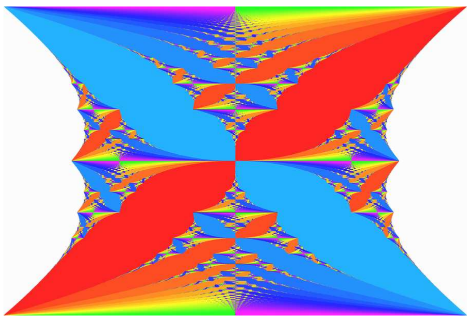

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Bloch orbitals

- Lattice-periodical Hamiltonian (no **macroscopic** **B** field); 2d, single band, spinless electrons

$$
\begin{aligned}
H|\psi_{\mathbf{k}}\rangle &= \varepsilon_{\mathbf{k}}|\psi_{\mathbf{k}}\rangle \\
H_{\mathbf{k}}|u_{\mathbf{k}}\rangle &= \varepsilon_{\mathbf{k}}|u_{\mathbf{k}}\rangle \qquad |u_{\mathbf{k}}\rangle = \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}}|\psi_{\mathbf{k}}\rangle \quad H_{\mathbf{k}} = \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}} H \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}
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- Berry curvature $(\vartheta, \varphi) \longrightarrow (k_x, k_y)$:

$$\Omega(\mathbf{k}) = i \left(\langle \partial_{k_x} u_{\mathbf{k}} | \partial_{k_y} u_{\mathbf{k}} \rangle - \langle \partial_{k_y} u_{\mathbf{k}} | \partial_{k_x} u_{\mathbf{k}} \rangle \right)$$

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Chern number

- BZ is a **closed** surface (2d torus). Gauss-Bonnet-Chern:

$$\frac{1}{2\pi}\int_{\mathrm{BZ}} d\mathbf{k}\;\mathbf{\Omega}(\mathbf{k}) = C_1 \in \mathbb{Z}$$

- Constant under deformations of the Hamiltonian insofar as the **gap does not close**

- 2D crystalline material with $C_1 \neq 0$:
  - Prototype of a **topological insulator**
  - Haldane **(1988)** proved that such a material **could exist**
  - This "simple" kind of topological insulators synthetized since **2013 onwards**

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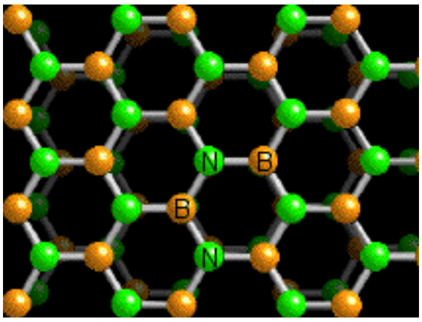
Hexagonal boron nitride (& graphene)



Topologically trivial: $C_1 = 0$.
Why?

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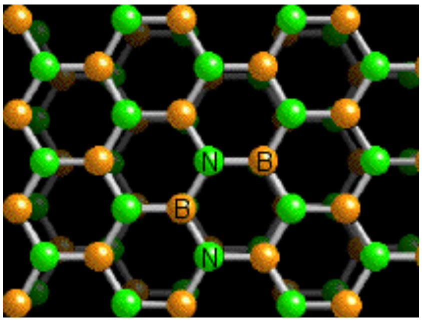

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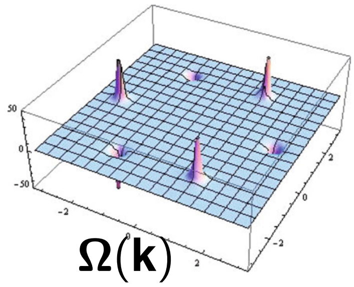

$\boldsymbol{\Omega}(\mathbf{k})$

Symmetry properties

- Time-reversal symmetry $\rightarrow \boldsymbol{\Omega}(\mathbf{k}) = -\boldsymbol{\Omega}(-\mathbf{k})$
- Inversion symmetry $\rightarrow \boldsymbol{\Omega}(\mathbf{k}) = \boldsymbol{\Omega}(-\mathbf{k})$

- Need to introduce **"some magnetism"**
- Solution: a **staggered** magnetic field

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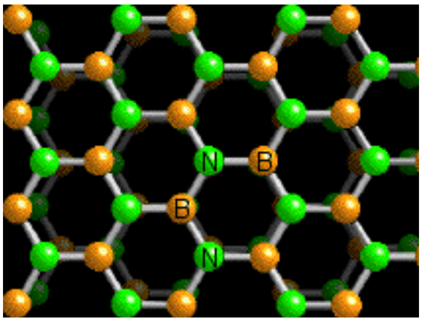

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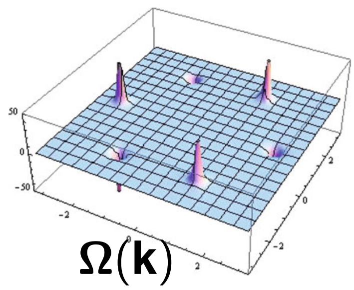

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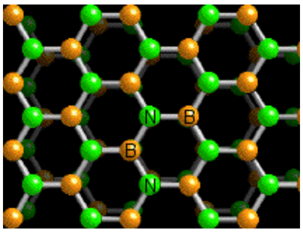
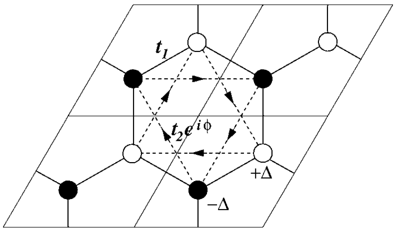
- Inversion symmetry $\rightarrow \boldsymbol{\Omega}(\mathbf{k}) = \boldsymbol{\Omega}(-\mathbf{k})$

- Need to introduce **"some magnetism"**
- Solution: a **staggered** magnetic field

The “Haldanium” paradigm (F.D.M. Haldane, 1988)

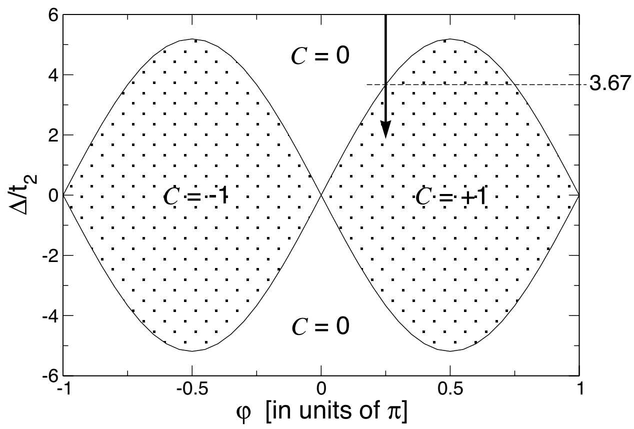


+ **staggered** B field



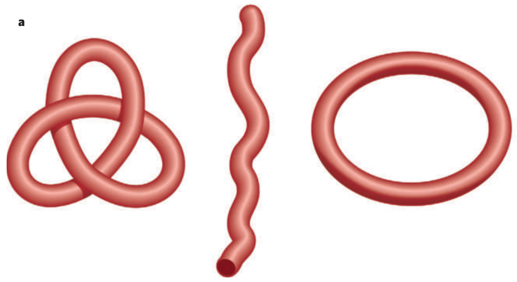
Tight-binding parameters:

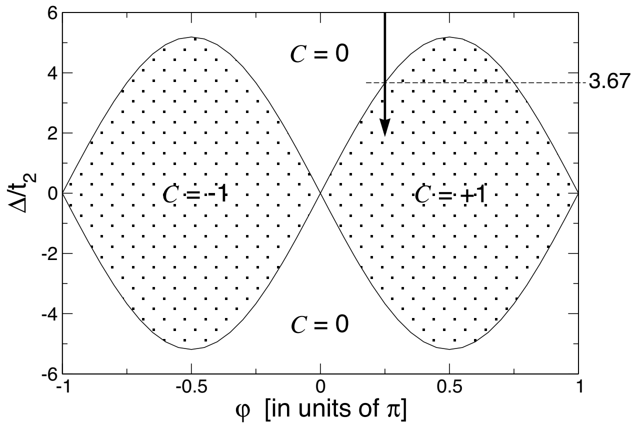
- 1st-neighbor hopping t_1
- staggered onsite $\pm\Delta$
- complex 2nd-neighbor $t_2 e^{i\phi}$



Phase diagram

Topological order



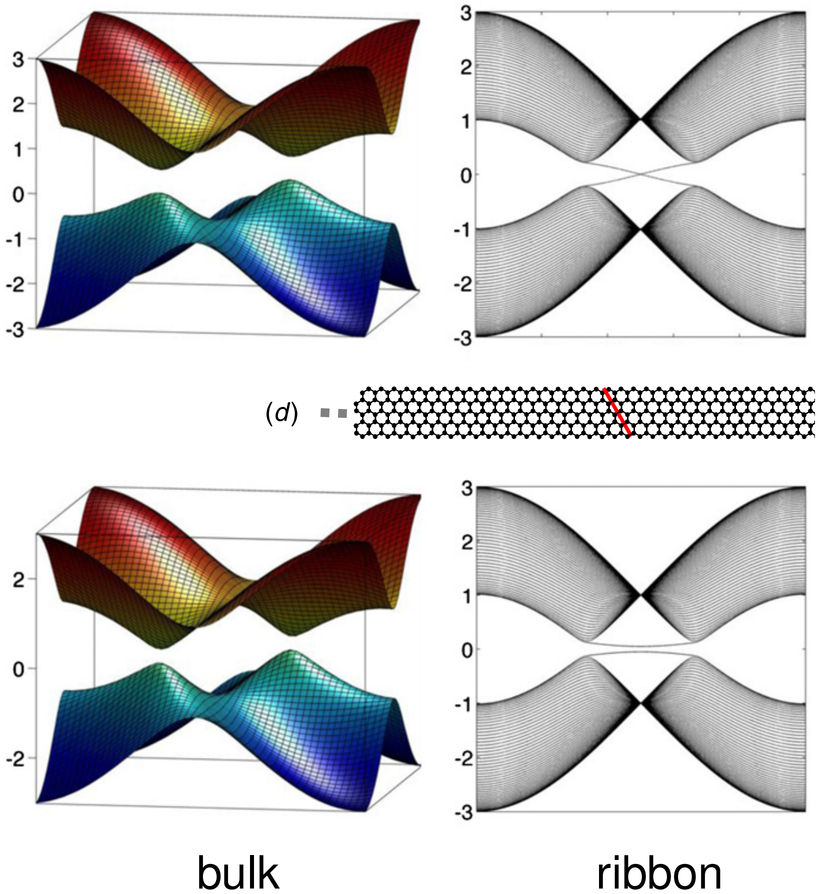


- Ground state wavefunctions differently "knotted" in **k** space
- Topological order very robust
- C_1 switched only via a metallic state: "cutting the knot"
- Displays quantum Hall effect at $\mathbf{B} = 0$

Bulk-boundary correspondence

$C_1 \neq 0$

$C_1 = 0$



Outline

Manifesto: **k** space vs. **r** space

- Periodic boundary conditions and **k** vectors are a (very useful) creation of our mind: they do not exist in nature.
- Topological order must be detected even:
  - Inside finite samples (e.g. bounded crystallites)
  - In noncrystalline samples
  - In macroscopically inhomogeneous samples (e.g. heterojunctions)
- In all such cases, the **k** vector does not make much sense

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Manifesto: **k** space vs. **r** space

- Is it possible to get rid of **k** vectors and to detect instead topological order **directly in r space**?

Manifesto: **k** space vs. **r** space

PHYSICAL REVIEW B **84**, 241106(R) (2011)

Mapping topological order in coordinate space

Raffaello Bianco and Raffaele Resta

Our “topological marker”

R. Bianco and R. Resta, Phys. Rev. B (RC) **84**, 241106 (2011)

- We design an operator $\mathcal{O}$, **explicitly** given in the Schrödinger representation: $\langle \mathbf{r}|\mathcal{O}|\mathbf{r}'\rangle$
- Our operator is well defined both for unbounded crystals and for bounded samples (e.g. crystallites)
- The diagonal $\langle \mathbf{r}|\mathcal{O}|\mathbf{r}\rangle$ has the meaning of **curvature per unit area** in $\mathbf{r}$ space

  …but **fluctuates** on a microscopic scale
- Its **trace per unit volume** in any macroscopically homogeneous region of the sample yields C_1

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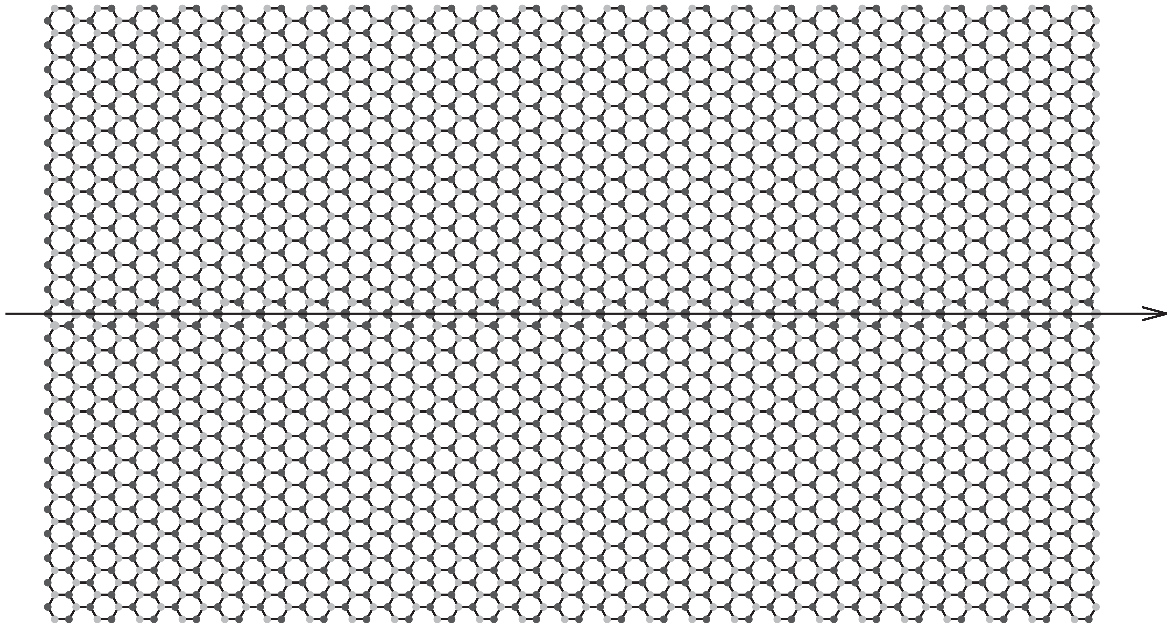
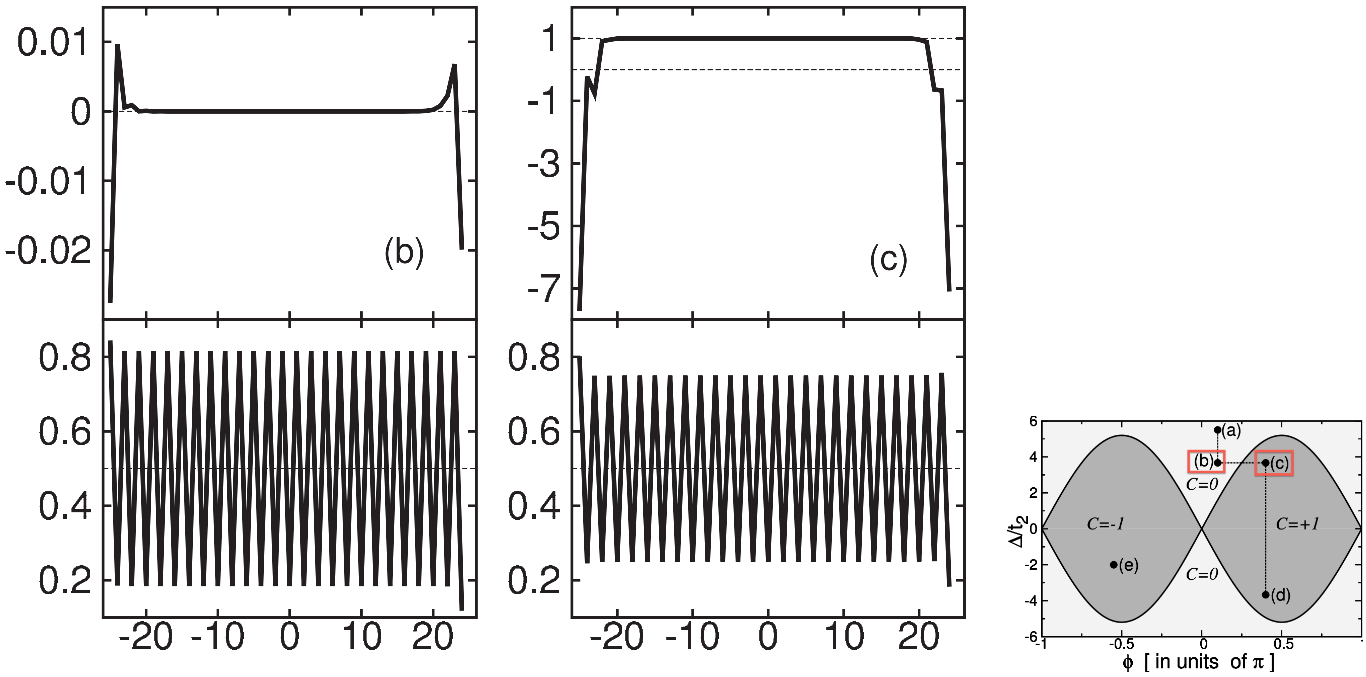
Haldanium flake (OBCs)



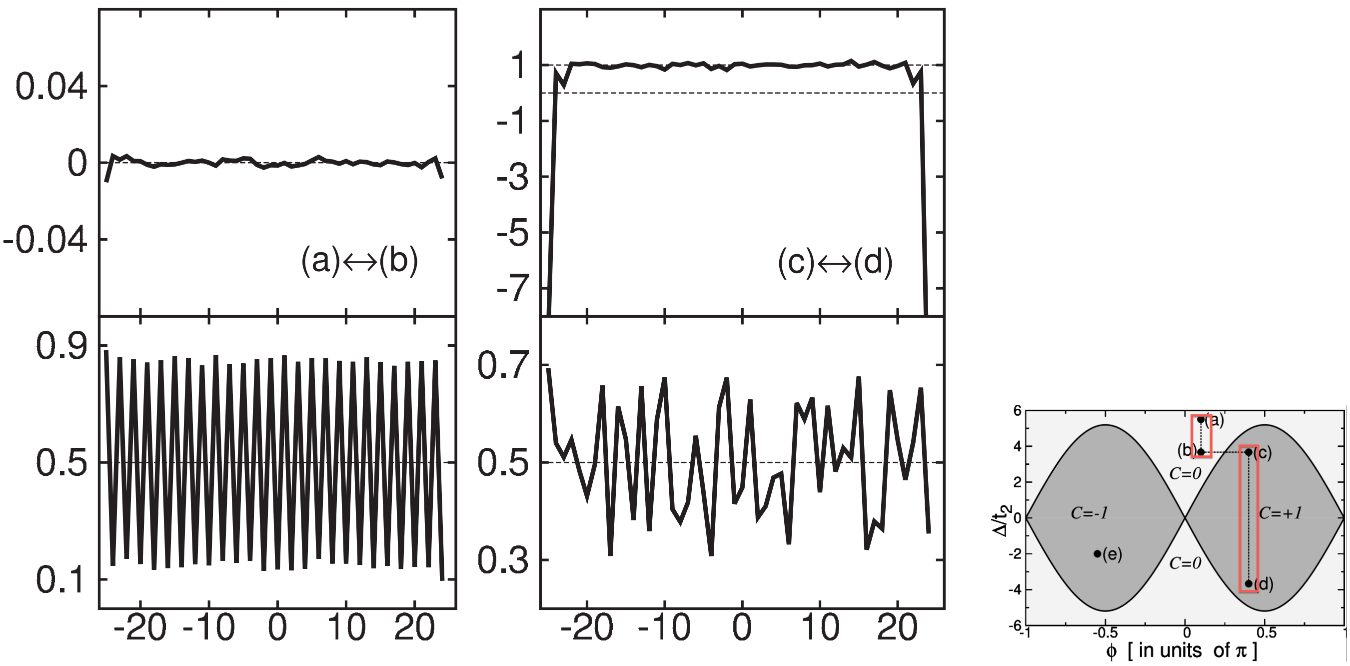
Sample of 2550 sites, line with 50 sites

Crystalline Haldanium (normal & Chern)



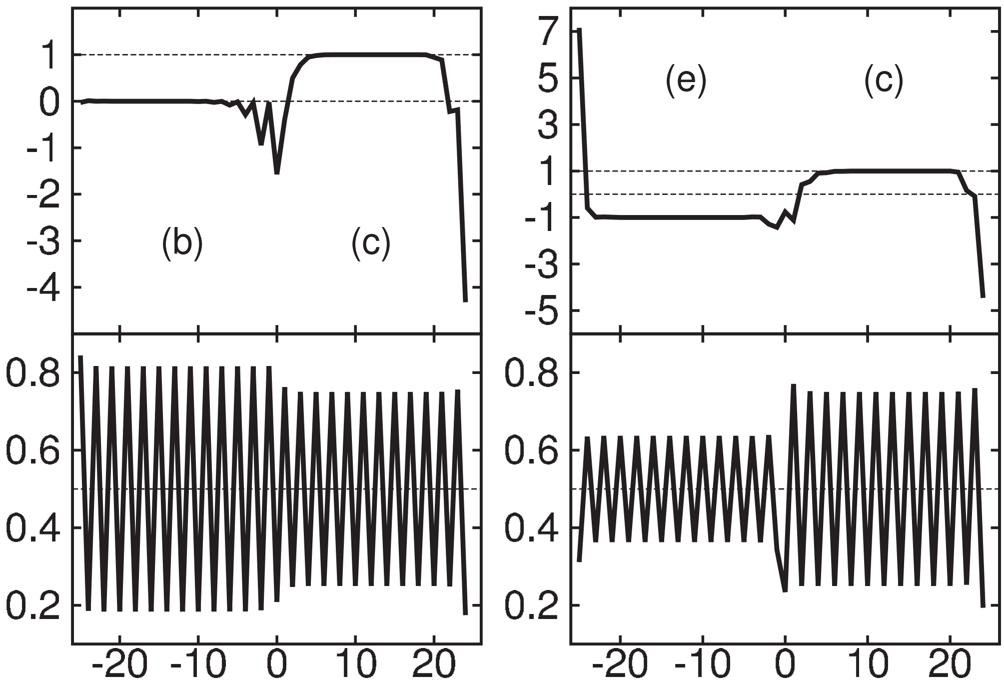
Topological marker (top); site occupancy (bottom)

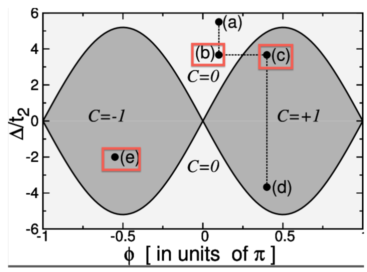
Haldanium alloy (normal & Chern)



Topological marker (top); site occupancy (bottom)

Haldanium heterojunctions





Topological marker (top); site occupancy (bottom)

Outline

Conclusions and perspectives

- Topological invariants and topological order
  Wave function “knotted” in **k** space
- Topological invariants are measurable integers
  Very robust (“topologically protected”)
  Most spectacular: quantum Hall effect
- Topological order without a *B* field: topological insulators
- Topological order is (also) a **local** property of the ground-state wave function: Our simulations