Topology and Electronic Structure: Introduction

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Outline

1. Geometry in nonrelativistic QM
2. What topology is about
3. Surface charge in insulators
4. Integer quantum Hall effect & TKNN invariant

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1 Geometry in nonrelativistic QM

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Aharonov-Bohm, 1959

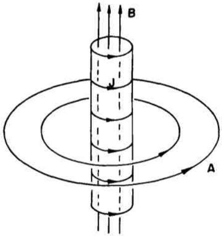

Fig. 15–6. The magnetic field and vector potential of a long solenoid.

Figure from Feynman, Vol. 2

Berry phase, 1984

- **Geometry** makes its debut in nonrelativistic quantum mechanics and in electronic structure
- Very simple concept, nonetheless missed by the founding fathers of QM in the 1920s and 1940s
- Nowadays in any modern elementary QM textbook

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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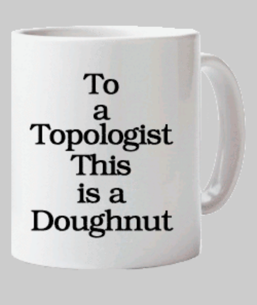
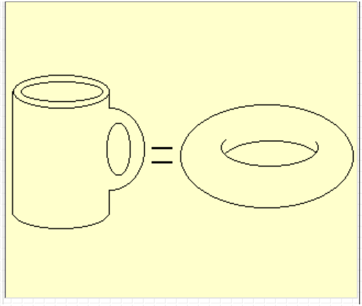
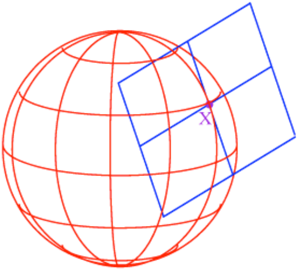
A coffee cup and a doughnut are the same





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

Gaussian curvature: sphere



In a local set of coordinates in the tangent plane

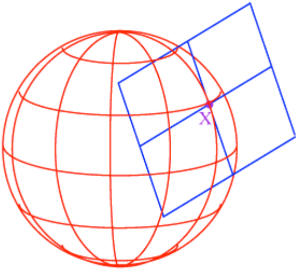
$$z = R - \sqrt{R^2 - x^2 - y^2} \simeq \frac{x^2 + y^2}{2R}$$

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

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

$$\frac{1}{2\pi} \int_S d\sigma \, K = 2$$

Gaussian curvature: sphere



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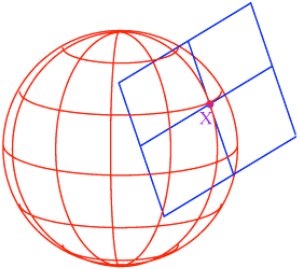

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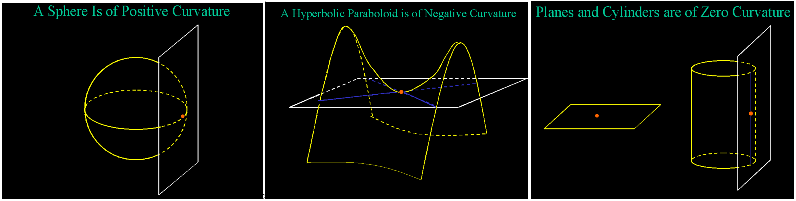
Positive and negative curvature



Smooth surface, local set of coordinates on the tangent plane

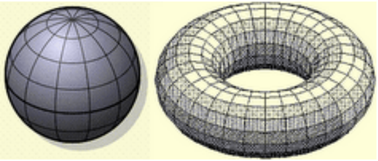
$$K = \det \begin{pmatrix} \frac{\partial^2 z}{\partial x^2} & \frac{\partial^2 z}{\partial x \partial y} \\ \frac{\partial^2 z}{\partial y \partial x} & \frac{\partial^2 z}{\partial y^2} \end{pmatrix}$$

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



$g = 0$ $g = 1$

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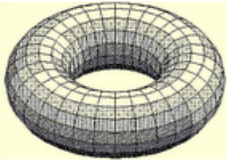
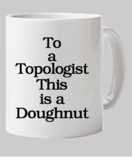

$g = 0$ $\quad g = 1$ $\quad g = 1$ $\quad g = 2$

Nonsmooth surfaces: Polyhedra

Euler characteristic $\chi = V - E + F$

Name	Image	Vertices V	Edges E	Faces F	Euler characteristic: $V - E + F$
Tetrahedron		4	6	4	**2**
Hexahedron or cube		8	12	6	**2**
Octahedron		6	12	8	**2**
Dodecahedron		20	30	12	**2**
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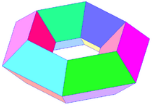

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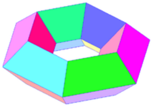

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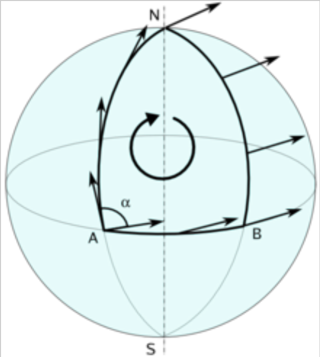
Parallel transport on a curved surface



Parallel transport of a vector around a closed loop (from A to N to B and back to A) on the sphere. The angle by which it twists, α, is proportional to the area inside the loop.

Angular mismatch α on a closed contour
= integral of the Gaussian curvature on the surface

Technical name:
Holonomy

Curvature
= Angular mismatch per unit area

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Quantization of surface charge

(Theorem discovered & rediscovered several times 1966-1986)

Theorem:

- If the bulk is an insulating & **centrosymmetric** crystal
- If the surface is also insulating
- Then the surface charge per unit surface area is $Q = e/2 \times \text{integer} \in \mathbb{Z}$

Consequence:

- Among the Q values dictated by topology, Nature chooses the minimum energy one:
  - In 3d solids $Q = 0$: **even polar surfaces are neutral!** .... provided they are insulating
  - In quasi-1d (polymers) $Q \neq 0$ may occur

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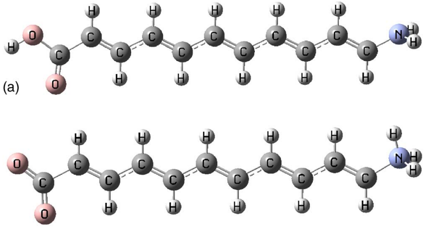
How the theorem works: Polyacetylene



Centrosymmetric bulk:

Two different
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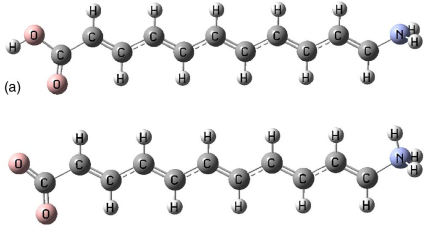

Centrosymmetric bulk:

Two different
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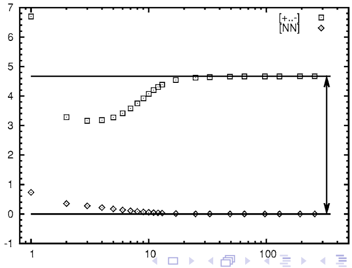
Dipole per cell = Qa

Here:
either $Q = 0$ or $Q = 1$



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Debut of topology in electronic structure

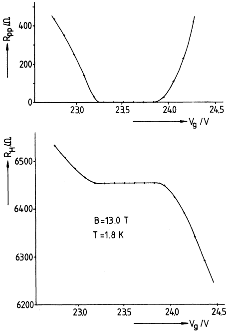

Figure from von Klitzing et al. (1980).

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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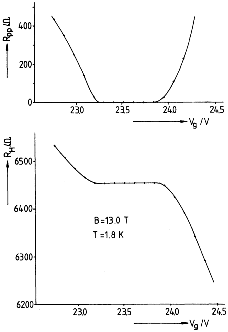

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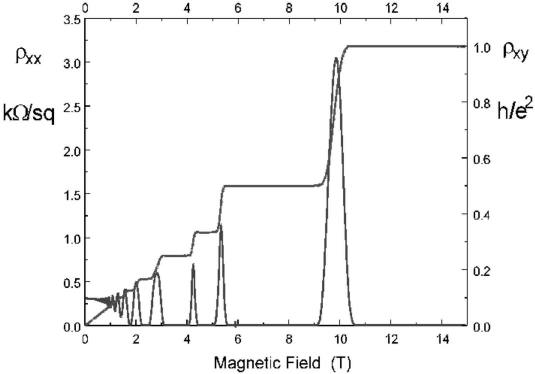
More recent experiments

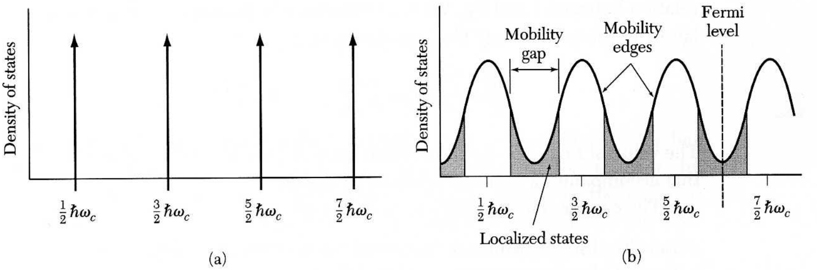


- Plateaus accurate to nine decimal figures
- In the plateau regions $\rho_{xx} = 0$ **and** $\sigma_{xx} = 0$: "quantum Hall insulator"

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)



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