Topological Order in Electronic Wavefunctions

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Outline

1. What topology is about
2. Elements of Berryology
3. Chern insulators
4. Noncrystalline insulators
5. Chern number as a cumulant moment in **r** space
6. Conclusions

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1 What topology is about

2 Elements of Berryology

3 Chern insulators

4 Noncrystalline insulators

5 Chern number as a cumulant moment in **r** space

6 Conclusions

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 to ferret out the meaning of physical concepts!)

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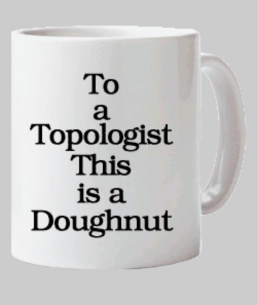
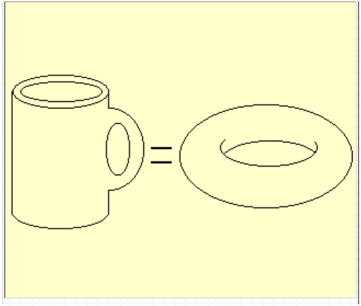
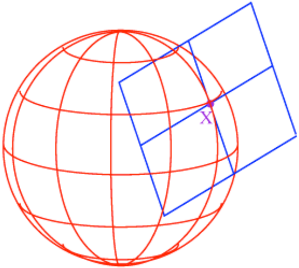
A coffee cup and a doughnut are the same





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

Gaussian curvature: sphere



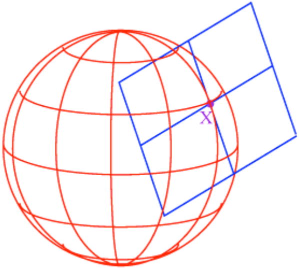
In a local set of coordinates in the tangent plane

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

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

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

Gaussian curvature: sphere



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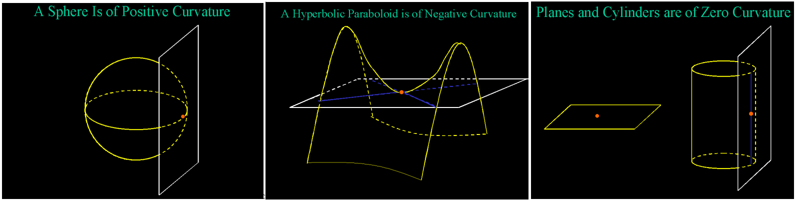
Positive and negative curvature



Smooth surface, local set of coordinates on the tangent plane

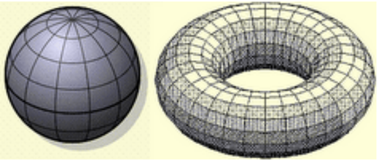
$$K = \det \begin{pmatrix} \frac{\partial^2 z}{\partial x^2} & \frac{\partial^2 z}{\partial x \partial y} \\ \frac{\partial^2 z}{\partial y \partial x} & \frac{\partial^2 z}{\partial y^2} \end{pmatrix}$$

Gauss-Bonnet theorem

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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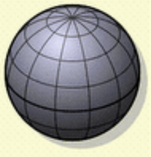

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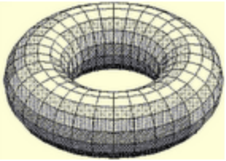

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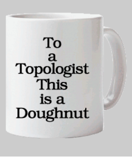
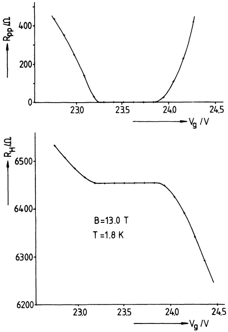


$g = 1$

$g = 2$

Debut of topology in electronic structure



Discovery of 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.
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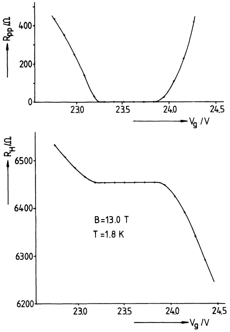

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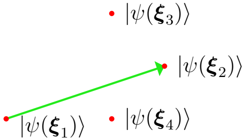
Basics

Parametric Hamiltonian, non degenerate ground state

$$H(\xi)|\psi(\xi)\rangle = E(\xi)|\psi(\xi)\rangle \qquad \text{parameter } \xi\text{: “slow variable”}$$



$$e^{-i\Delta\varphi_{12}} = \frac{\langle\psi(\boldsymbol{\xi}_1)|\psi(\boldsymbol{\xi}_2)\rangle}{|\langle\psi(\boldsymbol{\xi}_1)|\psi(\boldsymbol{\xi}_2)\rangle|}$$

$$\Delta\varphi_{12} = -\,\mathrm{Im}\,\log\,\langle\psi(\boldsymbol{\xi}_1)|\psi(\boldsymbol{\xi}_2)\rangle$$

$$\gamma = \Delta\varphi_{12} + \Delta\varphi_{23} + \Delta\varphi_{34} + \Delta\varphi_{41}$$

$$= -\,\mathrm{Im}\,\log\,\langle\psi(\boldsymbol{\xi}_1)|\psi(\boldsymbol{\xi}_2)\rangle\langle\psi(\boldsymbol{\xi}_2)|\psi(\boldsymbol{\xi}_3)\rangle\langle\psi(\boldsymbol{\xi}_3)|\psi(\boldsymbol{\xi}_4)\rangle\langle\psi(\boldsymbol{\xi}_4)|\psi(\boldsymbol{\xi}_1)\rangle$$

Gauge-invariant!

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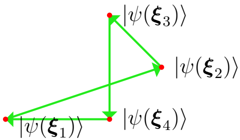

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Gauge-invariant!

Berry connection & Berry curvature

For a **differentiable** gauge:

- Berry connection $\boldsymbol{\mathcal{A}}(\boldsymbol{\xi}) = i \langle \psi(\boldsymbol{\xi}) | \nabla_{\boldsymbol{\xi}} \psi(\boldsymbol{\xi}) \rangle$
  - real, nonconservative vector field
  - gauge-dependent
  - "geometrical" vector potential

- Berry curvature
  $\boldsymbol{\Omega}(\boldsymbol{\xi}) = \nabla_{\boldsymbol{\xi}} \times \boldsymbol{\mathcal{A}}(\boldsymbol{\xi}) = i \langle \nabla_{\boldsymbol{\xi}} \psi(\boldsymbol{\xi}) | \times | \nabla_{\boldsymbol{\xi}} \psi(\boldsymbol{\xi}) \rangle$
  - gauge-invariant (hence observable)
  - geometric analog of a magnetic field

Berry phase

- Loop integral of the Berry connection on a closed path:

$$\gamma = \oint_C \mathcal{A}(\xi) \cdot d\xi$$

  - Berry phase, gauge invariant **only modulo** 2π
  - corresponds to **measurable** effects

- If $C = \partial\Sigma$ is the boundary of Σ, then (Stokes th.):

$$\gamma = \oint_{\partial\Sigma} \mathcal{A}(\xi) \cdot d\xi = \int_{\Sigma} d\sigma\, \mathbf{\Omega}(\xi) \cdot \hat{\mathbf{n}}$$

  - requires Σ to be simply connected
  - requires $\mathcal{A}$ to be regular on Σ
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A simple example: Two level system

$$
\begin{aligned}
H(\boldsymbol{\xi}) &= \boldsymbol{\xi} \cdot \vec{\sigma} \qquad \text{nondegenerate for } \boldsymbol{\xi} \neq 0 \\
&= \xi \left(\sin\vartheta \cos\varphi \, \sigma_x + \sin\vartheta \sin\varphi \, \sigma_y + \cos\vartheta \, \sigma_z\right)
\end{aligned}
$$

lowest eigenvalue $-\xi$

lowest eigenvector $|\psi(\vartheta,\varphi)\rangle = \begin{pmatrix} \sin\frac{\vartheta}{2} e^{-i\varphi} \\ -\cos\frac{\vartheta}{2} \end{pmatrix}$

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\begin{aligned}
\mathcal{A}_\vartheta &= i\langle\psi|\partial_\vartheta\psi\rangle = 0 \\
\mathcal{A}_\varphi &= i\langle\psi|\partial_\varphi\psi\rangle = \sin^2\frac{\vartheta}{2} \\
\boldsymbol{\Omega} &= \partial_\vartheta\mathcal{A}_\varphi - \partial_\varphi\mathcal{A}_\vartheta = \frac{1}{2}\sin\vartheta
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- Ω gauge invariant
- What about $\mathcal{A}$? **Obstruction!**

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Integrating the Berry curvature

- Gauss-Bonnet-Chern theorem (1940):

$$\frac{1}{2\pi}\int_{S^2} \mathbf{\Omega}(\xi)\cdot\mathbf{n}\; d\sigma = \text{topological integer} \in \mathbb{Z}$$

- Integrating $\Omega(\vartheta,\varphi)$ over $[0,\pi]\times[0,2\pi]$:

$$\frac{1}{2\pi}\int d\vartheta d\varphi\; \frac{1}{2}\sin\vartheta = 1 \qquad \text{Chern number } C_1$$

- Measures the singularity at $\xi = 0$ (monopole)

- Berry phase on any closed curve C on the sphere:

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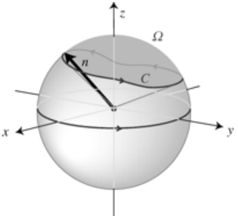

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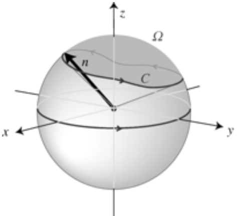

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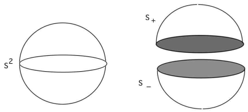
The sphere as the sum of two half spheres



$$
\begin{aligned}
2\pi C_1 &= \int_{S^2} \mathbf{\Omega}(\xi)\cdot\mathbf{n}\, d\sigma \\
&= \int_{S_+} \mathbf{\Omega}(\xi)\cdot\mathbf{n}\, d\sigma + \int_{S_-} \mathbf{\Omega}(\xi)\cdot\mathbf{n}\, d\sigma
\end{aligned}
$$

Stokes: $\displaystyle \int_{S_\pm} \mathbf{\Omega}(\xi)\cdot\mathbf{n}\, d\sigma = \pm \oint_C \mathcal{A}_\pm(\xi)\cdot d\xi$

$$
\int_{S^2} \mathbf{\Omega}(\xi)\cdot\mathbf{n}\, d\sigma = \oint_C \mathcal{A}_+(\xi)\cdot d\xi - \oint_C \mathcal{A}_-(\xi)\cdot d\xi
$$

Gauge choice: $\mathcal{A}_-(\xi)$ regular in the lower hemisphere: hence it has an **obstruction** in the upper hemisphere

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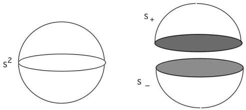

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Bloch orbitals (noninteracting electrons in this talk)

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

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H|\psi_{\mathbf{k}}\rangle &= \varepsilon_{\mathbf{k}}|\psi_{\mathbf{k}}\rangle \\
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\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 connection and curvature $(\xi \rightarrow \mathbf{k})$:

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\mathcal{A}(\mathbf{k}) &= i\langle u_{\mathbf{k}}|\nabla_{\mathbf{k}} u_{\mathbf{k}}\rangle \\
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- BZ (or reciprocal cell) is a **closed** surface: 2d torus
  Topological invariant:

$$
C_1 = \frac{1}{2\pi}\int_{\mathrm{BZ}} d\mathbf{k}\; \Omega(\mathbf{k}) \qquad \text{Chern number}
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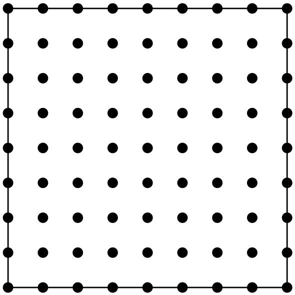
Computing the Chern number

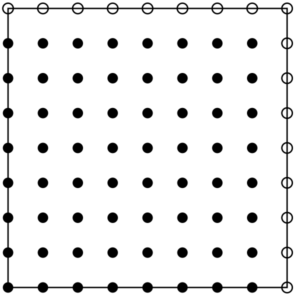
Discretized reciprocal cell



Computing the Chern number

Discretized reciprocal cell

Periodic gauge choice:
where is the obstruction?



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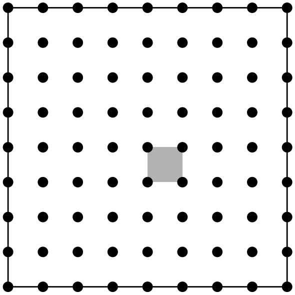

Curvature $\equiv$ Berry phase per unit (reciprocal) area
Berry phase on a small square:

$$\gamma = -\text{Im}\log \langle u_{\mathbf{k}_1}|u_{\mathbf{k}_2}\rangle\langle u_{\mathbf{k}_2}|u_{\mathbf{k}_3}\rangle\langle u_{\mathbf{k}_3}|u_{\mathbf{k}_4}\rangle\langle u_{\mathbf{k}_4}|u_{\mathbf{k}_1}\rangle$$

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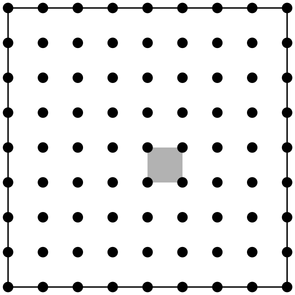

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Which branch of Im log?

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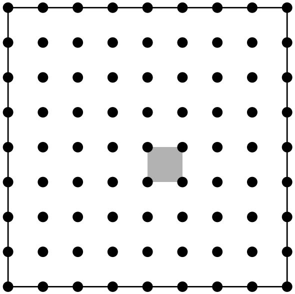

NonAbelian (many-band):

$$\gamma = -\text{Im}\,\log\,\det\, S(\mathbf{k}_1,\mathbf{k}_2)S(\mathbf{k}_2,\mathbf{k}_3)S(\mathbf{k}_3,\mathbf{k}_4)S(\mathbf{k}_4,\mathbf{k}_1)$$

$$S_{nn'}(\mathbf{k}_s,\mathbf{k}_{s'}) = \langle u_{n\mathbf{k}_s} | u_{n\mathbf{k}_{s'}} \rangle$$

Outline

1 What topology is about

2 Elements of Berryology

3 Chern insulators

4 Noncrystalline insulators

5 Chern number as a cumulant moment in **r** space

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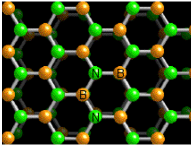
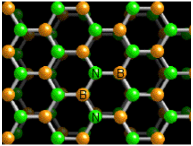
Hexagonal boron nitride (& graphene)



Topologically trivial: $C_1 = 0$.
Why?

- Need to break time-reversal invariance!
- B field in the quantum Hall effect (TKNN invariant)
- What about graphene?

Hexagonal boron nitride (& graphene)



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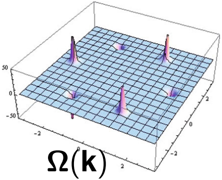
Why?

Symmetry properties

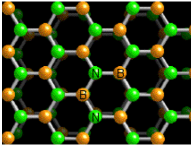
- Time-reversal symmetry $\rightarrow \boldsymbol{\Omega}(\mathbf{k}) = -\boldsymbol{\Omega}(-\mathbf{k})$
- Inversion symmetry $\rightarrow \boldsymbol{\Omega}(\mathbf{k}) = \boldsymbol{\Omega}(-\mathbf{k})$



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

- Need to break time-reversal invariance!
- B field in the quantum Hall effect (TKNN invariant)
- What about graphene?

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



+ **staggered** B field

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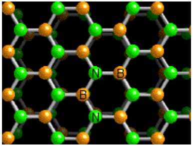

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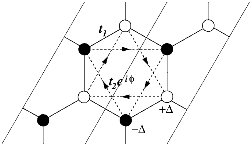
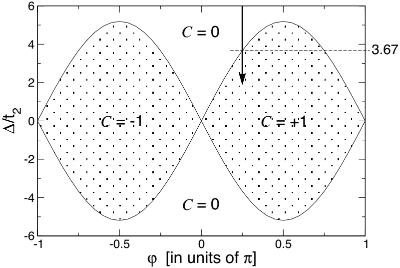


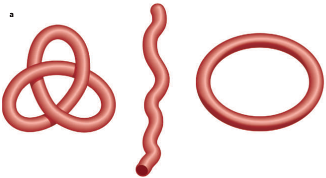
Tight-binding parameters:

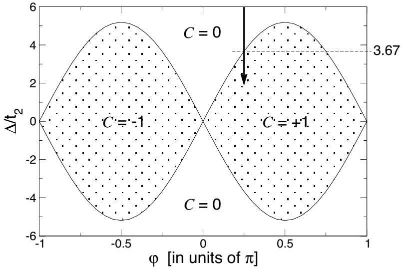
- 1st-neighbor hopping t_1
- staggered onsite $\pm\Delta$
- complex 2nd-neighbor $t_2 e^{i\phi}$



Phase diagram

Topological order



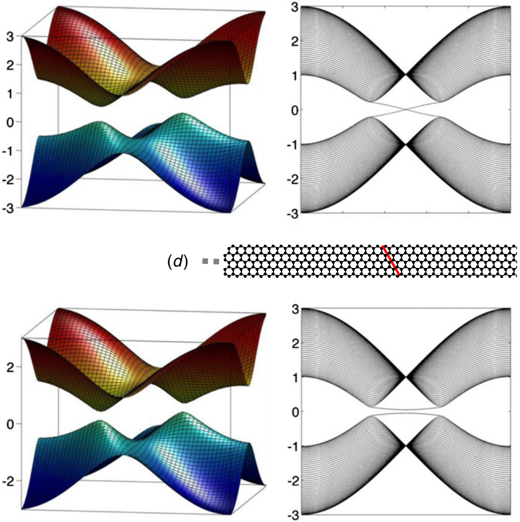


- Ground state wavefunctions differently “knotted” in **k** space
- Topological order very robust
- C_1 switched only via a metallic state: “cutting the knot”
- Displays quantum Hall effect at $B = 0$

Bulk-boundary correspondence

$C_1 \neq 0$

$C_1 = 0$



bulk

ribbon

Wannier functions do not exist when $C_1 \neq 0$
(Thouless, 1984)

- Proof by absurd. If WFs exist then

$$|\psi_{\mathbf{k}}\rangle = \sum_{\mathbf{R}} e^{i\mathbf{k}\cdot\mathbf{R}} |\mathbf{R}\rangle$$

- This implies

$$|\psi_{\mathbf{k}+\mathbf{G}}\rangle = |\psi_{\mathbf{k}}\rangle \quad \text{(so called “periodic gauge”)}$$

- When $C_1 \neq 0$ a periodic gauge in the whole BZ does not exist: **topological obstruction**

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Simulation by T. Thonhauser & D. Vanderbilt, 2006

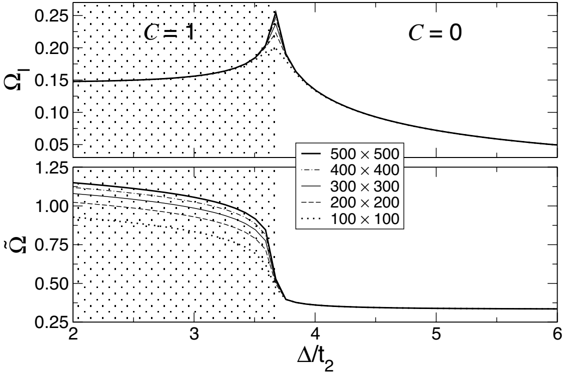

FIG. 8. Gauge-independent part Ω_I and gauge-dependent part $\tilde{\Omega}$ of the spread functional for the Haldane model as a function of the **k**-mesh density.

Chern insulators

- Besides Haldanium (a very popular computational material), do Chern insulators exist in nature?
- Discovery announced at the 2012 APS March Meeting, not confirmed by any preprint yet (to my knowledge)
- Also called **QAHE** (quantum anomalous Hall effect). Why?
- Nonexotic ferromagnetic metals in 3d (Ni, Co, Fe) show **AHE**: Hall effect in zero B field.
  Nonquantized: Berry curvature integrated within the Fermi volume.

Time-reversal symmetric topological insulators

- In 2d:
  - Kane-Mele model Hamiltonian, 2005
  - A novel invariant, two-valued ($\mathbb{Z}_2$)
  - Zero order picture: two copies of the Haldane model
  - Discovered: $Hg_xCd_{1-x}Te$ quantum wells, 2007 (L. Molenkamp & al.)
- In 3d:
  - Predicted by Fu, Kane, and Mele in 2007
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2012 O. E. Buckley Condensed Matter Physics Prize

- “For the **theoretical prediction and experimental observation** of the quantum spin Hall effect, opening the field of topological insulators”

- Charles L. Kane (U. Pennsylvania)
  Laurens W. Molenkamp (U. Würzburg, Germany)
  Shoucheng Zhang (Stanford U.)

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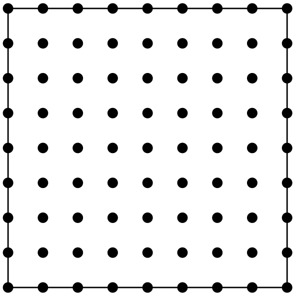
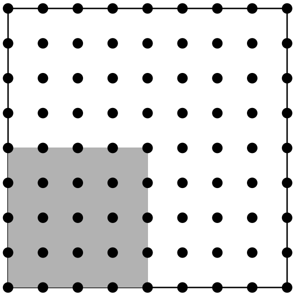
Computing the Chern number



Computing the Chern number

Cell doubling:

- Reciprocal cell **reduced** fourfold
- # of states **increased** fourfold
- the states are **the same**
- C_1 invariant



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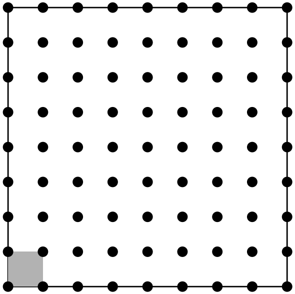

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Down to the very minimum:

- One state on many loops $\rightarrow$ Many states on a single loop
- The gauge is now periodical throughout:
  Where is the obstruction?
- Eventually, C_1 is a $\mathbf{k} = 0$ property!

Interpretation of the single point formula

- In the large supercell limit

$$C_1 = \frac{1}{2\pi} \int_{\mathrm{BZ}} d\mathbf{k}\ \mathbf{\Omega}(\mathbf{k}) \quad \rightarrow \quad \frac{1}{2\pi} \frac{(2\pi)^2}{A_c} \mathbf{\Omega}(0)$$

Chern number $\rightarrow$ curvature per unit sample area:
no integration

- $\Omega(0)$ is a linear response of the ground state to an infinitesimal "twist" or "flux" in the many-body Hamiltonian:

$$\hat{H}(\mathbf{k}) = \frac{1}{2m_e} \sum_{i=1}^{N} |\mathbf{p}_i + \frac{e}{c}\mathbf{A}(\mathbf{r}_i) + \hbar\mathbf{k}|^2 + \hat{V}$$

$$\mathbf{\Omega}(0) = i \sum_{n=1}^{N} (\ \langle \partial_{k_1} u_{n0} | \partial_{k_2} u_{n0} \rangle - \langle \partial_{k_2} u_{n0} | \partial_{k_1} u_{n0} \rangle\ )$$

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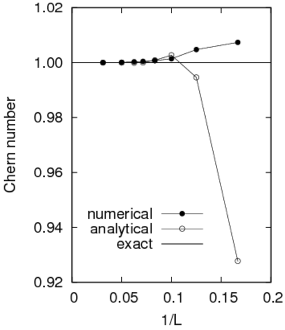
Convergence with supercell size
(D. Ceresoli & R.R. 2007)

Chern number as a function of the supercell size, evaluated using the single-point formulas for the Haldane model Hamiltonian. The largest L corresponds to 2048 sites in the supercell.



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

- Is topological order purely a **k** space business?
- Can I detect topological order in a finite sample ("open boundary conditions")?
- Can I detect topological order in a macroscopically inhomogeneous sample?
- The one-body density matrix (ground state projector):
  - determines the ground state (independent electrons)
  - embeds the information about topological order
  - is "shortsighted" (© by W. Kohn)
  - hence.......

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Shortsightedness (noninteracting spinless electrons)

$P(\mathbf{r}, \mathbf{r}')$ ground-state projector

- $P(\mathbf{r}, \mathbf{r}')$ uniquely determines the ground state
- If we look at $P(\mathbf{r}, \mathbf{r}')$ in the **bulk of a sample** the boundary conditions (either open or periodic) become irrelevant

- Asymptotic behavior of $|P(\mathbf{r}, \mathbf{r}')|$ for $|\mathbf{r} - \mathbf{r}'| \to \infty$:
  - Power law in metals
  - Exponential in insulators
  - Gaussian in the IQHE

Insulating vs. metallic ground state

The "localization tensor", a.k.a. second cumulant moment of the electron distribution

- Definition within OBCs:

$$\langle r_\alpha r_\beta \rangle_c = \frac{1}{2N} \int d\mathbf{r} d\mathbf{r}' \, (\mathbf{r}-\mathbf{r}')_\alpha (\mathbf{r}-\mathbf{r}')_\beta \, |P(\mathbf{r},\mathbf{r}')|^2$$

  - Always well defined (**r** operator harmless within OBCs)
  - Intensive (size-consistent)
  - **Real symmetric**
  - Original theory for correlated wavefunctions

- Identical transformation:

$$Q(\mathbf{r},\mathbf{r}') = \delta(\mathbf{r}-\mathbf{r}') - P(\mathbf{r},\mathbf{r}') \qquad \langle r_\alpha r_\beta \rangle_c = \frac{1}{N} \mathrm{Tr}_{\text{all space}} \{ r_\alpha P r_\beta Q \}$$

- What about the thermodynamic limit?
  - $\sum_\alpha \langle r_\alpha r_\alpha \rangle_c$ diverges in metals
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Brillouin-zone integral

Switching to a crystalline solid (PBCs):

$$\langle r_\alpha r_\beta \rangle_c = \frac{1}{N} \mathrm{Tr}_{\text{all space}} \{ r_\alpha P r_\beta Q \} \quad \rightarrow \quad \frac{1}{N_c} \mathrm{Tr}_{\text{cell}} \{ r_\alpha P r_\beta Q \}$$

r operator harmless when sandwiched between P and Q

In terms of Bloch states $e^{i\mathbf{k}\cdot\mathbf{r}} u_{n\mathbf{k}}$ (in 2d):

$$\langle r_\alpha r_\beta \rangle_c = \frac{A_c}{(2\pi)^2 N_c} \int d\mathbf{k} \left(\sum_n \langle \partial_{k_\alpha} u_{n\mathbf{k}} | \partial_{k_\beta} u_{n\mathbf{k}} \rangle - \sum_{n,n'} \langle u_{n\mathbf{k}} | \partial_{k_\alpha} u_{n'\mathbf{k}} \rangle \langle \partial_{k_\beta} u_{n'\mathbf{k}} | u_{n\mathbf{k}} \rangle \right)$$

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Marzari-Vanderbilt

$$\sum_\alpha \langle r_\alpha r_\alpha \rangle_{\rm c} = \frac{1}{N_{\rm c}} \Omega_{\rm I}$$ MV gauge-invariant quadratic spread

Naturally endowed with an off-diagonal imaginary part:

$$\mathrm{Im}\ \langle r_1 r_2 \rangle_{\rm c} = \frac{A_c}{(2\pi)^2 N_{\rm c}} \mathrm{Im} \int d\mathbf{k} \sum_n \langle \partial_{k_1} u_{n\mathbf{k}} | \partial_{k_2} u_{n\mathbf{k}} \rangle$$

Chern number:

$$C_1 = -\frac{1}{\pi} \mathrm{Im} \int d\mathbf{k} \sum_n \langle \partial_{k_1} u_{n\mathbf{k}} | \partial_{k_2} u_{n\mathbf{k}} \rangle$$

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Metric-curvature tensor (2d, 1 band)

$$\mathcal{F}_{\alpha\beta}(\mathbf{k}) = \langle \partial_{k_\alpha} u_{\mathbf{k}} | \partial_{k_\beta} u_{\mathbf{k}} \rangle - \langle \partial_{k_\alpha} u_{\mathbf{k}} | u_{\mathbf{k}} \rangle \langle u_{\mathbf{k}} | \partial_{k_\beta} u_{\mathbf{k}} \rangle$$

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$$\begin{aligned} \Omega_{\mathrm{I}} &= \frac{A_c}{(2\pi)^2} \int_{\mathrm{BZ}} d\mathbf{k}\, [\, g_{xx}(\mathbf{k}) + g_{yy}(\mathbf{k}) \,] && \text{gauge-invariant spread} \\ C_1 &= \frac{1}{2\pi} \int_{\mathrm{BZ}} d\mathbf{k}\, \Omega(\mathbf{k}) && \text{Chern number} \end{aligned}$$

Whenever Ω_{I} is finite, C_1 is quantized

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Whenever Ω_I is finite, C_1 is quantized

Ω_I finite, but WFs do not exist
(Simulation by Thonhauser & Vanderbilt, 2006)

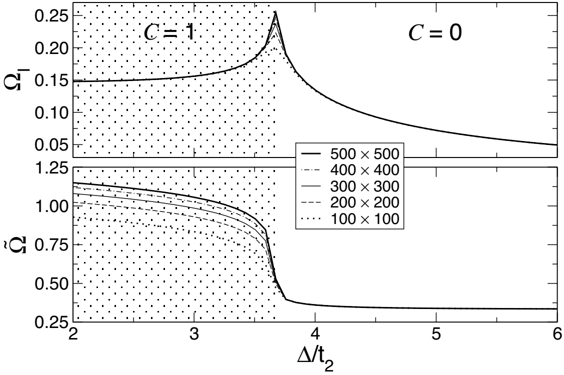

FIG. 8. Gauge-independent part Ω_I and gauge-dependent part $\tilde{\Omega}$ of the spread functional for the Haldane model as a function of the **k**-mesh density.

Chern number in terms of the density matrix

$$C_1 = -4\pi \frac{N_\mathrm{c}}{A_\mathrm{c}} \mathrm{Im}\, \langle r_1 r_2 \rangle_\mathrm{c} = -\frac{4\pi}{A_\mathrm{c}} \mathrm{Im}\ \mathrm{Tr}_\mathrm{cell}\{ r_1 P r_2 Q \}$$

- Proof for a lattice model: Kitaev 2006, Prodan 2009
  (Thanks to D. Vanderbilt)
- General proof **implicit** in Sgiarovello et al. 2001
- Imaginary part **quantized** whenever real part is **finite**
  (true even for correlated wavefunctions, e.g. FQHE)
- I started with a **real symmetric** tensor $\langle r_\alpha r_\beta \rangle_\mathrm{c}$:
  Where did the imaginary part sneak?

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From OBCs to PBCs

The apparently innocent ansatz:

$$\langle r_\alpha r_\beta \rangle_{\rm c} = \frac{1}{N} \text{Tr}_{\text{all space}} \{ r_\alpha P r_\beta Q \} \quad \rightarrow \quad \frac{1}{N_{\rm c}} \text{Tr}_{\text{cell}} \{ r_\alpha P r_\beta Q \}$$

- OBCs:
  - $\langle r_\alpha r_\beta \rangle_{\rm c}$ real symmetric Cartesian tensor
  - P projects on a finite-dimensional manifold
- PBCs:
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Numerical simulations

- Within OBCs:

$$\mathrm{Im}\ \mathrm{Tr}\{r_1 P r_2 P\} = \frac{1}{2i}\mathrm{Tr}\{\,[P r_1 P, P r_2 P]\,\} = 0$$

What happens?

Numerical simulations

- Within OBCs:

$$\mathrm{Im}\ \mathrm{Tr}\{r_1 P r_2 P\} = \frac{1}{2i}\mathrm{Tr}\{\,[P r_1 P, P r_2 P]\,\} = 0$$

  What happens?

- Answer: computer simulations on Haldanium, once more

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Mapping topological order in coordinate space

Raffaello Bianco and Raffaele Resta

Chern number as a local quantity

$$\operatorname{Im}\operatorname{Tr}\{r_1 P r_2 P\} = \frac{1}{2i}\operatorname{Tr}\{\,[P r_1 P, P r_2 P]\,\}$$

$$C_1 = -\frac{2\pi i}{A_c}\operatorname{Tr}_{\text{cell}}\{\,[P r_1 P, P r_2 P]\,\} \equiv -2\pi i \frac{1}{A_c}\int_{\text{cell}} d\mathbf{r}\,\langle \mathbf{r}|\,[P r_1 P, P r_2 P]\,|\mathbf{r}\rangle$$

C_1 **macroscopic average** of $\mathfrak{C}(\mathbf{r})$

$\mathfrak{C}(\mathbf{r}) = -2\pi i \langle \mathbf{r}|\,[P r_1 P, P r_2 P]\,|\mathbf{r}\rangle$ **"topological marker"**

Can also be interpreted as the **curvature per unit area**!

Last but not least: Boundary conditions **irrelevant**

Chern number as a local quantity

$$\text{Im}\,\text{Tr}\{r_1 P r_2 P\} = \frac{1}{2i}\text{Tr}\{\,[Pr_1 P, Pr_2 P]\,\}$$

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$\mathfrak{C}(\mathbf{r}) = -2\pi i \langle \mathbf{r}|\,[Pr_1 P, Pr_2 P]\,|\mathbf{r}\rangle$ **"topological marker"**

Can also be interpreted as the **curvature per unit area**!

Last but not least: Boundary conditions **irrelevant**

Chern number as a local quantity

$$\text{Im Tr}\{r_1 P r_2 P\} = \frac{1}{2i}\text{Tr}\{\, [Pr_1 P, Pr_2 P]\,\}$$

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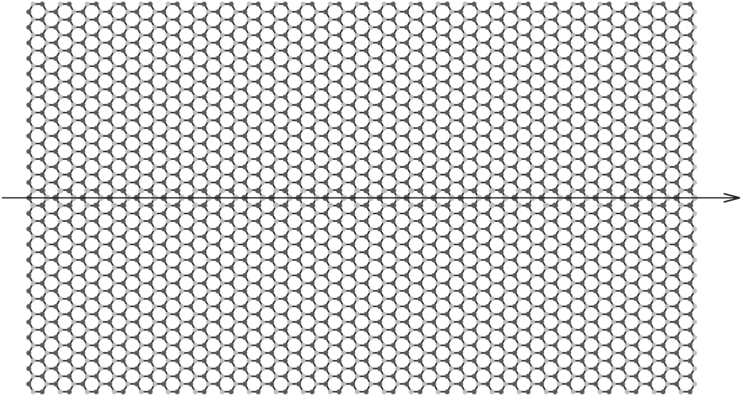
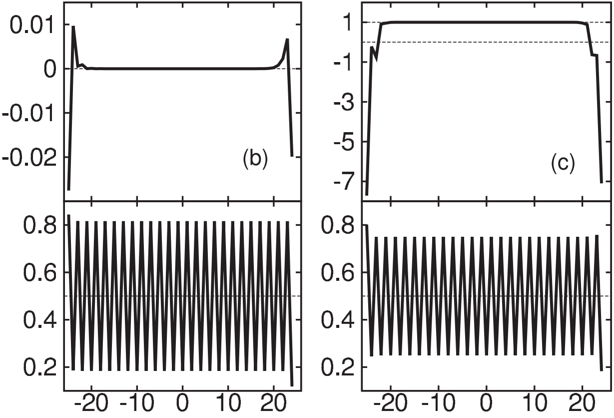
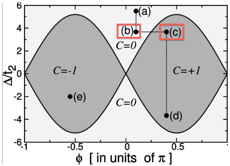
Haldanium flake (OBCs)



Sample of 2550 sites, line with 50 sites

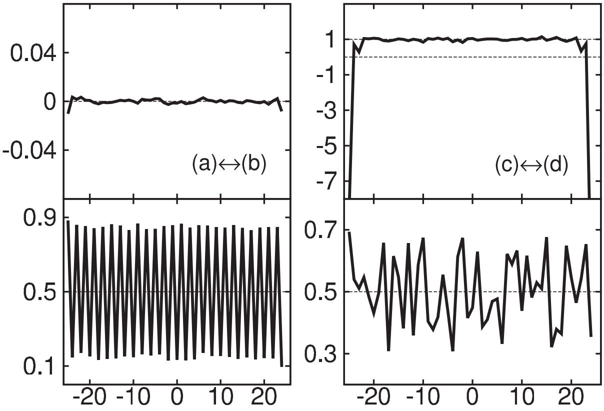
Crystalline Haldanium (normal & Chern)

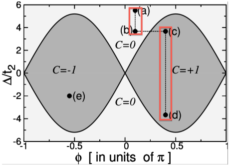




Topological marker (top); site occupancy (bottom)

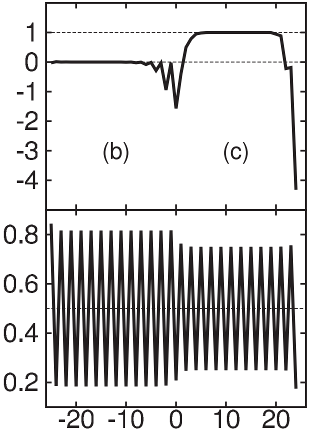
Haldanium alloy (normal & Chern)

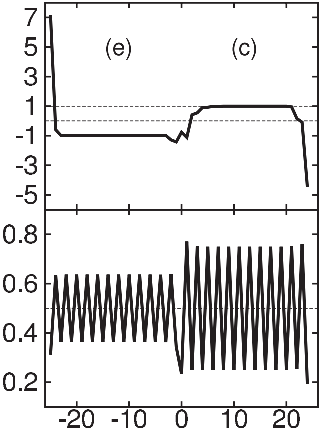


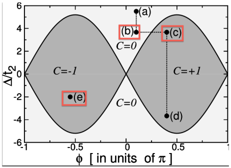


Topological marker (top); site occupancy (bottom)

Haldanium heterojunctions







Topological marker (top); site occupancy (bottom)

Outline

1 What topology is about

2 Elements of Berryology

3 Chern insulators

4 Noncrystalline insulators

5 Chern number as a cumulant moment in **r** space

6 Conclusions

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

- What about other kinds of topological order (e.g. $\mathbb{Z}_2$)?

Collaborators

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