Anomalous Hall conductivity (insulators and metals)

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Outline

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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}
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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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\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):

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

- 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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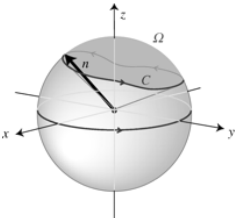

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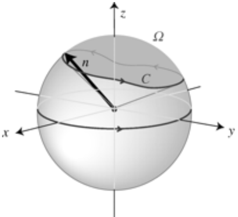

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Bloch orbitals (noninteracting electrons in this talk)

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

$$\begin{aligned} H|\psi_{\mathbf{k}}\rangle &= \varepsilon_{\mathbf{k}}|\psi_{\mathbf{k}}\rangle \\ H_{\mathbf{k}}|u_{\mathbf{k}}\rangle &= \varepsilon_{\mathbf{k}}|u_{\mathbf{k}}\rangle \end{aligned} \qquad |u_{\mathbf{k}}\rangle = \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}}|\psi_{\mathbf{k}}\rangle \quad H_{\mathbf{k}} = \mathrm{e}^{-i\mathbf{k}\cdot\mathbf{r}} H \mathrm{e}^{i\mathbf{k}\cdot\mathbf{r}}$$

- Berry connection and curvature $(\xi \to \mathbf{k})$:

$$\begin{aligned} \mathcal{A}(\mathbf{k}) &= i\langle u_{\mathbf{k}}|\nabla_{\mathbf{k}} u_{\mathbf{k}}\rangle \\ \Omega(\mathbf{k}) &= i\langle \nabla_{\mathbf{k}} u_{\mathbf{k}}| \times |\nabla_{\mathbf{k}} u_{\mathbf{k}}\rangle = -2\,\mathrm{Im}\,\langle \partial_{k_x} u_{\mathbf{k}}|\partial_{k_y} u_{\mathbf{k}}\rangle \end{aligned}$$

- 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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Many-band insulator (n_b occupied bands)

- Berry connection:

$$\mathcal{A}_\alpha(\mathbf{k}) = i \sum_{j=1}^{n_\mathrm{b}} \langle u_{j\mathbf{k}} | \partial_\alpha u_{j\mathbf{k}} \rangle$$

- Metric-curvature tensor of the occupied manifold:

$$\begin{aligned} \mathcal{F}_{\alpha\beta}(\mathbf{k}) &= \sum_{j=1}^{n_\mathrm{b}} \langle \partial_\alpha u_{j\mathbf{k}} | \partial_\beta u_{j\mathbf{k}} \rangle \\ &- \sum_{j,j'=1}^{n_\mathrm{b}} \langle \partial_\alpha u_{j\mathbf{k}} | u_{j'\mathbf{k}} \rangle \langle u_{j'\mathbf{k}} | \partial_\beta u_{j\mathbf{k}} \rangle \end{aligned}$$

Metric and curvature of the occupied manifold

- Quantum metric:

$$g_{\alpha\beta}(\mathbf{k}) = \mathrm{Re}\ \mathcal{F}_{\alpha\beta}(\mathbf{k})$$

- Berry curvature:

$$\boldsymbol{\Omega}_{\alpha\beta}(\mathbf{k}) = -2\ \mathrm{Im}\ \mathcal{F}_{\alpha\beta}(\mathbf{k}) = -2\ \mathrm{Im}\ \sum_{j=1}^{n_b} \langle \partial_\alpha u_{j\mathbf{k}} | \partial_\beta u_{j\mathbf{k}} \rangle$$

- Curvature useful for **metals** as well:

$$\Omega_{\alpha\beta}(\mathbf{k}) = -2\ \mathrm{Im}\ \sum_j f(\mu - \epsilon_{j\mathbf{k}})\ \langle \partial_\alpha u_{j\mathbf{k}} | \partial_\beta u_{j\mathbf{k}} \rangle$$

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$\Omega_{\rm I}$ as a bulk observable

I. Souza, T. Wilkens, and R. M. Martin, Phys. Rev. B **62**, 1666 (2000)

- Gauge-invariant quadratic spread of the WFs

$$\Omega_{\rm I} = V_{\rm cell} \sum_{\alpha} \int \frac{d\mathbf{k}}{(2\pi)^d}\, g_{\alpha\alpha}(\mathbf{k})$$

- SWM sum rule for the **longitudinal conductivity** of a band insulator:

$$\Omega_{\rm I} = \frac{\hbar V_{\rm cell}}{\pi e^2} \int_{\epsilon_{\rm g}/\hbar}^{\infty} \frac{d\omega}{\omega} \sum_{\alpha} \mathrm{Re}\, \sigma_{\alpha\alpha}(\omega),$$

- What about **metals**?

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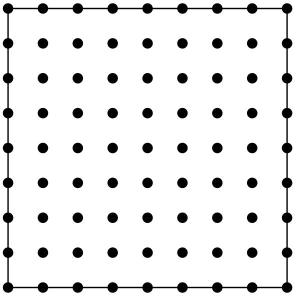
Computing the Chern number

Discretized reciprocal cell



Computing the Chern number

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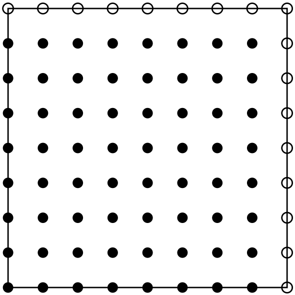
Periodic gauge choice:
where is the obstruction?



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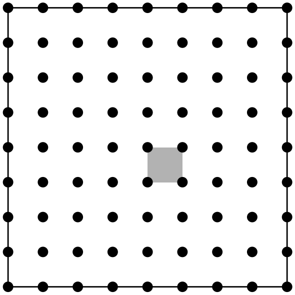

Curvature $\equiv$ Berry phase per unit (reciprocal) area
Berry phase on a small square:

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

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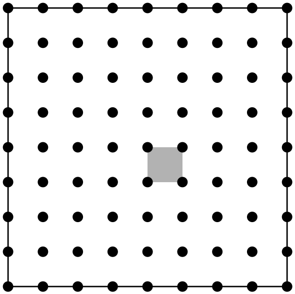

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Which branch of Im log?

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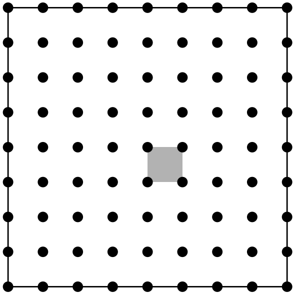


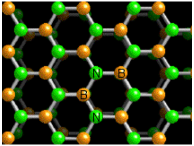
NonAbelian (many-band):

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

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

Outline

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?

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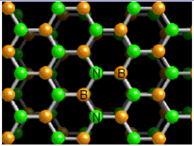

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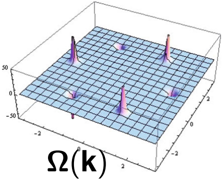

$\mathbf{\Omega}(\mathbf{k})$

Symmetry properties

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

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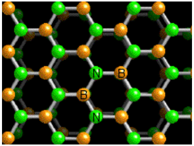
The “Haldanium” paradigm (F.D.M. Haldane, 1988)



+ **staggered** B field

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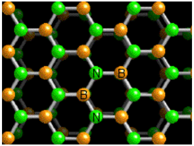

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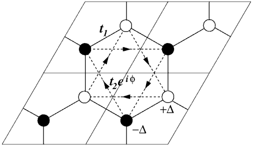
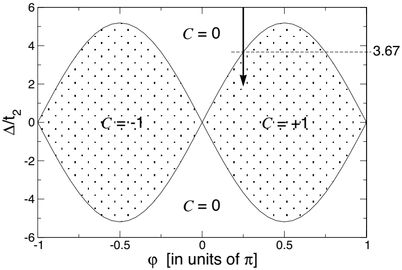


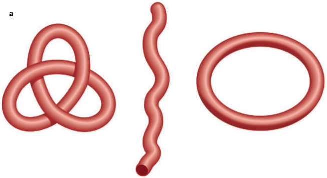
Tight-binding parameters:

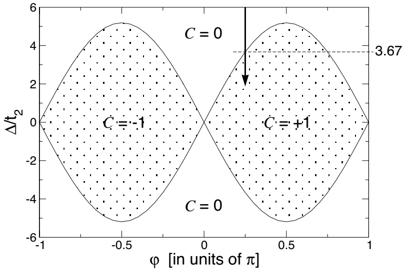
- 1st-neighbor hopping t_1
- staggered onsite $\pm\Delta$
- complex 2nd-neighbor $t_2 e^{i\phi}$



Phase diagram

Topological order



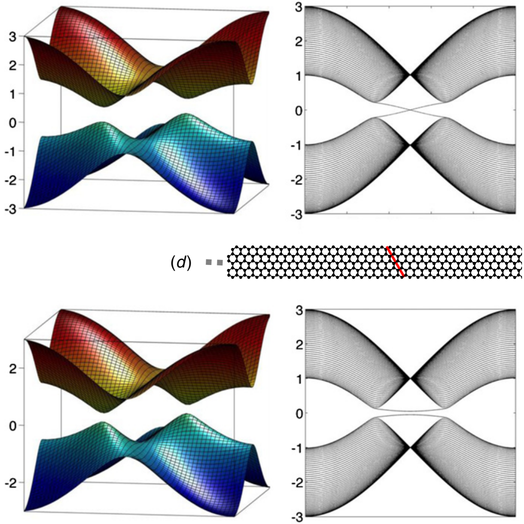


- Ground state wavefunctions differently "knotted" in **k** space
- Topological order very robust
- C_1 switched only via a metallic state: "cutting the knot"
- Displays quantum Hall effect at $B = 0$

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

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

- 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

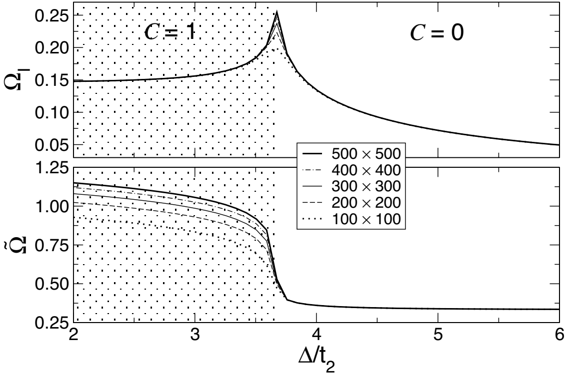

FIG. 8. Gauge-independent part Ω_I and gauge-dependent part $\tilde{\Omega}$ of the spread functional for the Haldane model as a function of the **k**-mesh density.

Chern insulators

- Besides Haldanium (a very popular computational material), do Chern insulators exist in nature?
- First synthetized in China in 2013
- 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.

Outline

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.)
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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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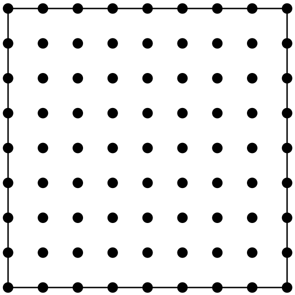
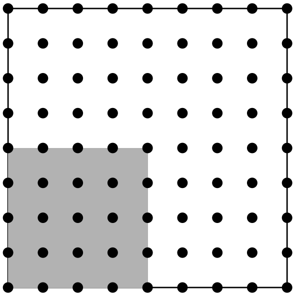
Computing the Chern number



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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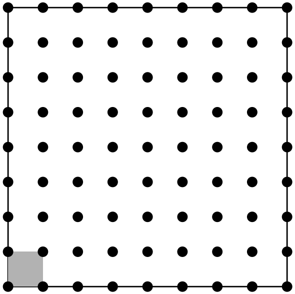

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Down to the very minimum:

- 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

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

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:

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

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

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

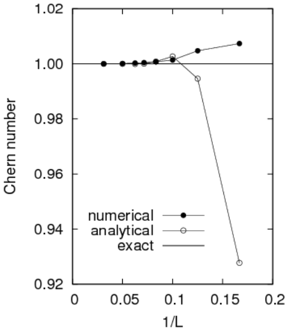
- $\mathbf{\Omega}(0)$ is a linear response of the ground state to an infinitesimal "twist" or "flux" in the many-body Hamiltonian:

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

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

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.



AHC and $\mathbf{M}$ as reciprocal-space integrals

- **Intrinsic term in anomalous Hall conductivity:**

$$\begin{aligned} \text{Re}\ \sigma^{(-)}_{\alpha\beta} &= -\frac{e^2}{\hbar}\int_{\mathrm{BZ}}\frac{d\mathbf{k}}{(2\pi)^d}\,\mathbf{\Omega}_{\alpha\beta}(\mathbf{k}) \\ &= \frac{2e^2}{\hbar}\sum_{\varepsilon_{j\mathbf{k}}<\mu}\int_{\mathrm{BZ}}\frac{d\mathbf{k}}{(2\pi)^d}\ \text{Im}\ \langle\partial_\alpha u_{j\mathbf{k}}|\partial_\beta u_{j\mathbf{k}}\rangle \end{aligned}$$

- Extrinsic terms:
  - Necessarily present in metals
  - Absent in insulators:
    Quantum anomalous Hall effect (QAHE)

- **Orbital magnetization:**

$$M_\gamma = \frac{e}{2\hbar c}\varepsilon_{\gamma\alpha\beta}\sum_{\varepsilon_{j\mathbf{k}}<\mu}\int_{\mathrm{BZ}}\frac{d\mathbf{k}}{(2\pi)^d}\ \text{Im}\ \langle\partial_\alpha u_{j\mathbf{k}}|\left(H_{\mathbf{k}}+\epsilon_{j\mathbf{k}}-2\mu\right)|\partial_\beta u_{j\mathbf{k}}\rangle$$

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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.
- **Genuine bulk properties** should also be measurable:
  - 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 any sense!
- Is it possible to get rid of **k** vectors and provide instead a **geometrical marker** directly in **r** space?

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Bounded samples with square-integrable orbitals

- One-body density matrix, a.k.a. ground-state projector:

$$\mathcal{P} = \sum_{\epsilon_j < \mu} |\varphi_j\rangle\langle\varphi_j| \quad \text{(spinless)}$$

- $\mathcal{P}$ allows to evaluate **any** ground-state observable (for independent electrons)

- Tensor fields in **r**-space:

$$\begin{aligned} \mathfrak{F}_{\alpha\beta}(\mathbf{r}) &= \operatorname{Im} \langle \mathbf{r} | \mathcal{P} [r_\alpha, \mathcal{P}] [r_\beta, \mathcal{P}] | \mathbf{r} \rangle \\ \mathfrak{M}_{\alpha\beta}(\mathbf{r}) &= \operatorname{Im} \langle \mathbf{r} | |\mathcal{H} - \mu| [r_\alpha, \mathcal{P}] [r_\beta, \mathcal{P}] | \mathbf{r} \rangle . \end{aligned}$$

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Geometrical observables as traces per unit volume

- Anomalous Hall conductivity:

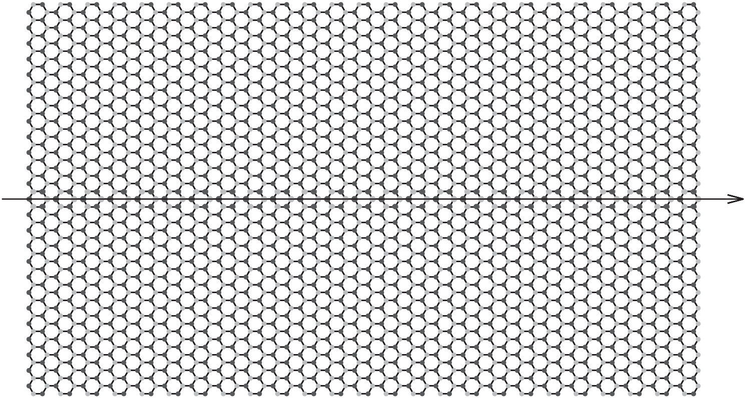
$$\sigma^{(-)}_{\alpha\beta} = -\frac{2e^2}{\hbar} \mathrm{Im}\,\mathrm{Tr}_V \{\mathfrak{F}_{\alpha\beta}\} \quad \text{(insulators \textbf{and} metals)}$$

- Orbital magnetization:

$$M_\gamma = \frac{e}{2\hbar c} \varepsilon_{\gamma\alpha\beta} \mathrm{Tr}_V \{\mathfrak{M}_{\alpha\beta}\} \quad \text{(insulators \textbf{and} metals)}$$

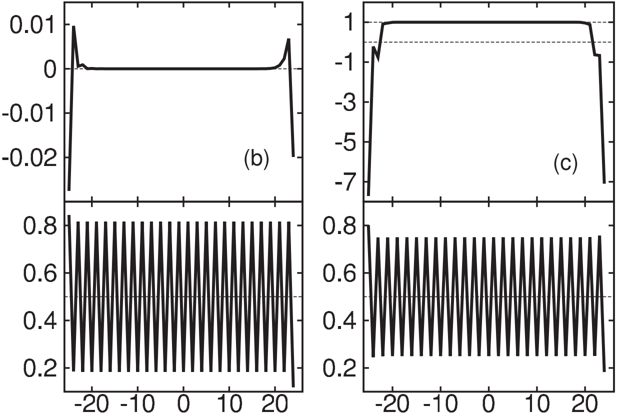
Outline

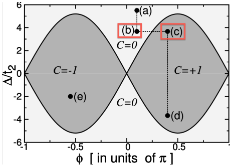
Haldanium flake (OBCs)



Sample of 1190 sites

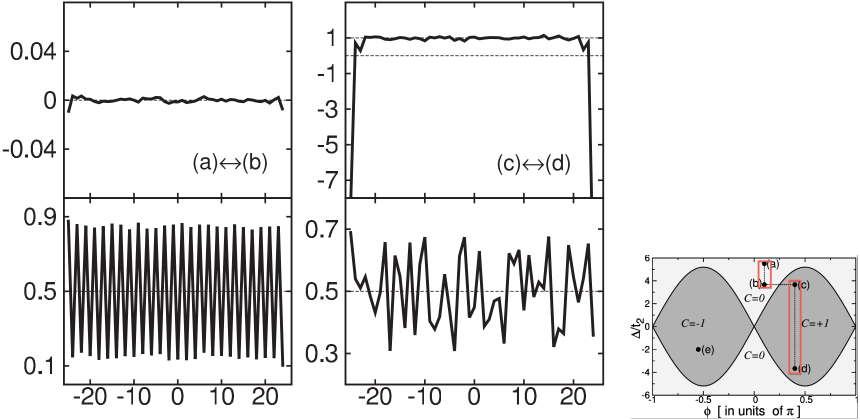
Normal insulator & Chern insulator (crystalline)





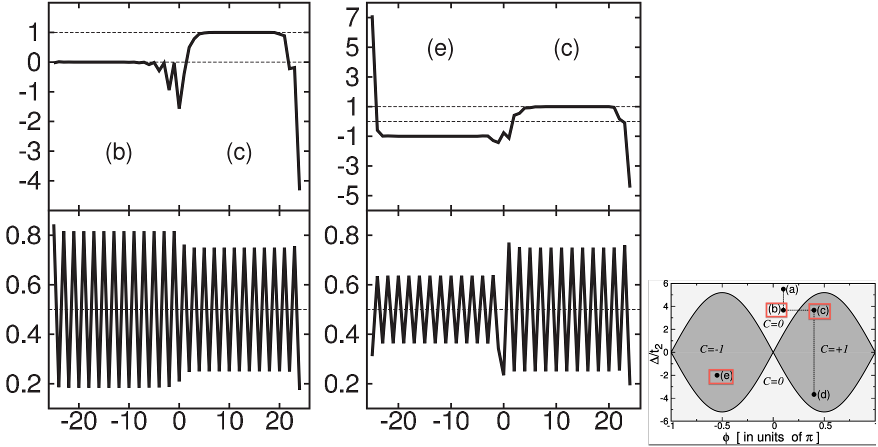
Topological marker (top); site occupancy (bottom)

Haldanium alloy (normal & Chern)



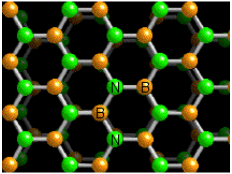
Topological marker (top); site occupancy (bottom)

Haldanium heterojunctions

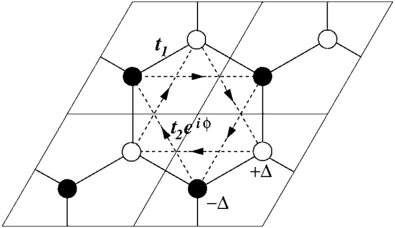


Topological marker (top); site occupancy (bottom)

Metallic Haldanium

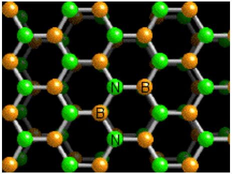


+ **"some magnetism"**



- Zero flux per cell (no Landau levels!)
- Insulating (either trivial or **topological**) at half filling
- **Metallic** at any other filling

Metallic Haldanium



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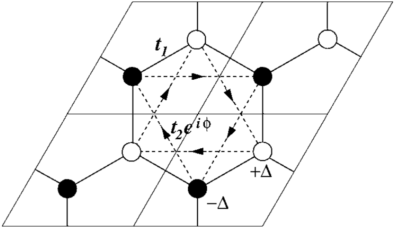

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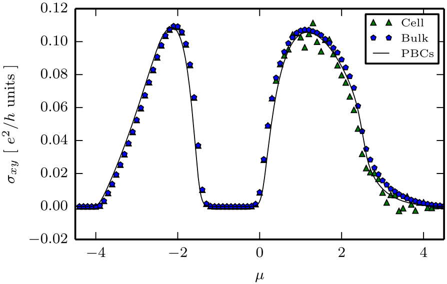
AHC in metals

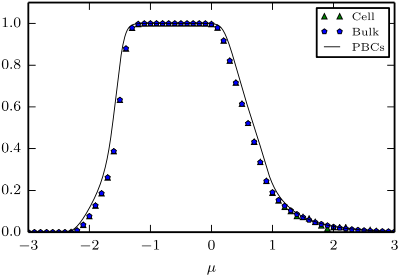
- Extrinsic mechanisms:
  - Side jump
  - Skew scattering
- Since the early 2000's
  - An important contribution is intrinsic
  - Geometrical property of the ground state (Fermi-volume integral of the Berry curvature)
  - **Nonquantized** version of QAHE in insulators
- We have proved that it is **local** in **r**-space

AHC as a function of the Fermi level
A. Marrazzo and R. Resta, Phys. Rev. B **95**, 121114(R) (2017)

- **Solid line:**
  Usual **k**-space expression (Fermi-volume integral)
- **Symbols:** Our **r**-space "geometrical marker"



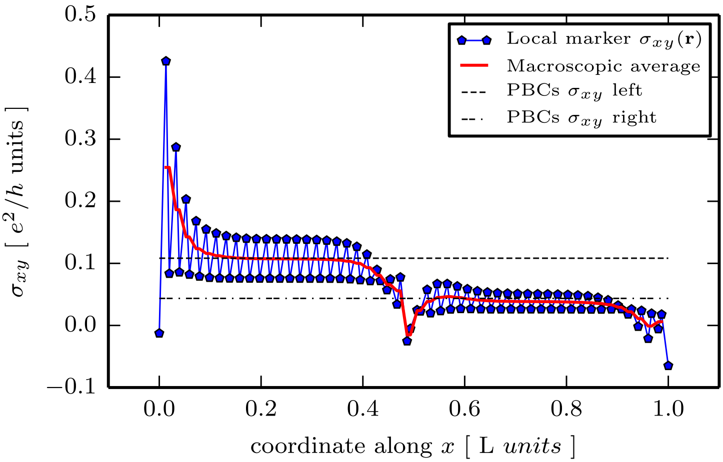
Trivial at half filling



Topological at half filling

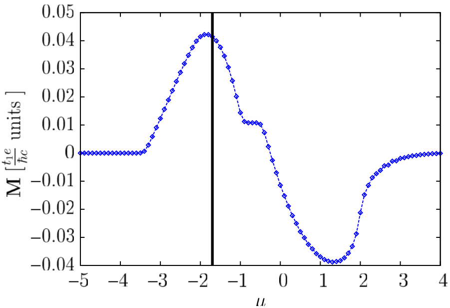
AHC in Haldanium metal/metal heterojunctions

A. Marrazzo and R. Resta, Phys. Rev. B **95**, 121114(R) (2017)



Orbital magnetization a a function of the Fermi level

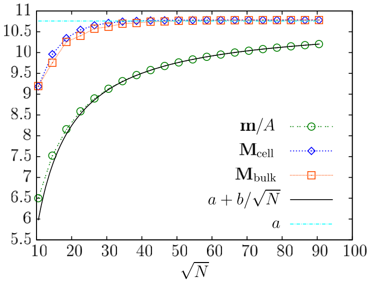
A. Marrazzo and R. Resta, Phys. Rev. Lett. **116**, 137201 (2016)



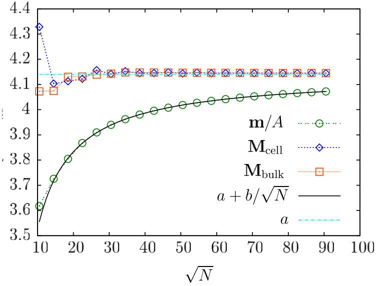
At convergence all formulas coincide:

- **Textbook formula:** $\frac{1}{2cV}\int d\mathbf{r}\;\mathbf{r}\times\mathbf{j}^{(\mathrm{micro})}(\mathbf{r})$
- $M_\gamma = -\frac{ie}{2\hbar c}\varepsilon_{\gamma\alpha\beta}\int_{\mathrm{FV}} d\mathbf{k}\,\langle\partial_\alpha u_{j\mathbf{k}}|\,(H_\mathbf{k}+\epsilon_{j\mathbf{k}}-2\mu)\,|\partial_\beta u_{j\mathbf{k}}\rangle$
- **Our novel formula:** $\frac{e}{2\hbar c}\varepsilon_{\gamma\alpha\beta}\mathrm{Tr}_V\,\{\mathfrak{M}_{\alpha\beta}\}$

Fast convergence in both insulator and metal



Insulator



Metal

- **$1/L$ convergence with size:** $\frac{1}{2cV}\int d\mathbf{r}\,\mathbf{r}\times\mathbf{j}^{(\text{micro})}(\mathbf{r})$
- **Much better convergence:** $\frac{e}{2\hbar c}\varepsilon_{\gamma\alpha\beta}\mathrm{Tr}_V\left\{\mathfrak{M}_{\alpha\beta}\right\}$

Why is our local **M** formula better than textbooks' one?

- **Textbooks:** bounded sample in the large-V limit:

$$
\begin{aligned}
M_\gamma &= \frac{1}{2cV}\varepsilon_{\gamma\alpha\beta}\int d\mathbf{r}\; r_\alpha\, j_\beta^{(\mathrm{micro})}(\mathbf{r}) \\
&= -\frac{e}{2cV}\varepsilon_{\gamma\alpha\beta}\sum_{\epsilon_j<\mu}\int d\mathbf{r}\;\langle\varphi_j|\, r_\alpha\, v_\beta\,|\varphi_j\rangle \\
&= -\frac{e}{2cV}\varepsilon_{\gamma\alpha\beta}\mathrm{Tr}\,\{\mathcal{P}\, r_\alpha v_\beta\}
\end{aligned}
$$

$$
\mathcal{P} = \sum_{\epsilon_j<\mu}|\varphi_j\rangle\langle\varphi_j|, \qquad v_\beta = \frac{i}{\hbar}[\mathcal{H}, r_\beta]
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- They provide the same **M** value at any finite V:
  Where is the **key difference**?

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\end{aligned}
$$

- The integral values are identical
- The **integrands** are very different
- Similar in spirit to an integration by parts

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- Integral dominated by **boundary contributions**:

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- Integral **boundary-insensitive**:

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- Integrand **lattice-periodical** in the bulk region:

$$\frac{1}{V}\int_{\text{sample}} d\mathbf{r}\ \langle \mathbf{r}|\,|\mathcal{H}-\mu|\,[r_\alpha,\mathcal{P}]\,[r_\beta,\mathcal{P}]\,|\mathbf{r}\rangle$$

$$\simeq \frac{1}{V_{\text{cell}}}\int_{\text{cell}} d\mathbf{r}\ \langle \mathbf{r}|\,|\mathcal{H}-\mu|\,[r_\alpha,\mathcal{P}]\,[r_\beta,\mathcal{P}]\,|\mathbf{r}\rangle$$

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