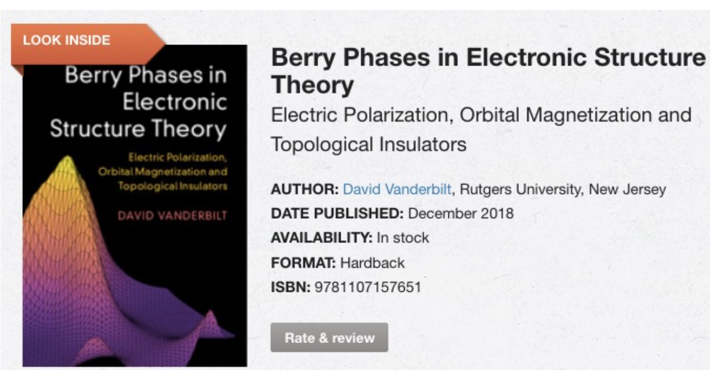
# Berry phases, Berry curvatures, and Hall conductivity




David Vanderbilt
Rutgers University

Slides available at https://is.gd/inFID2

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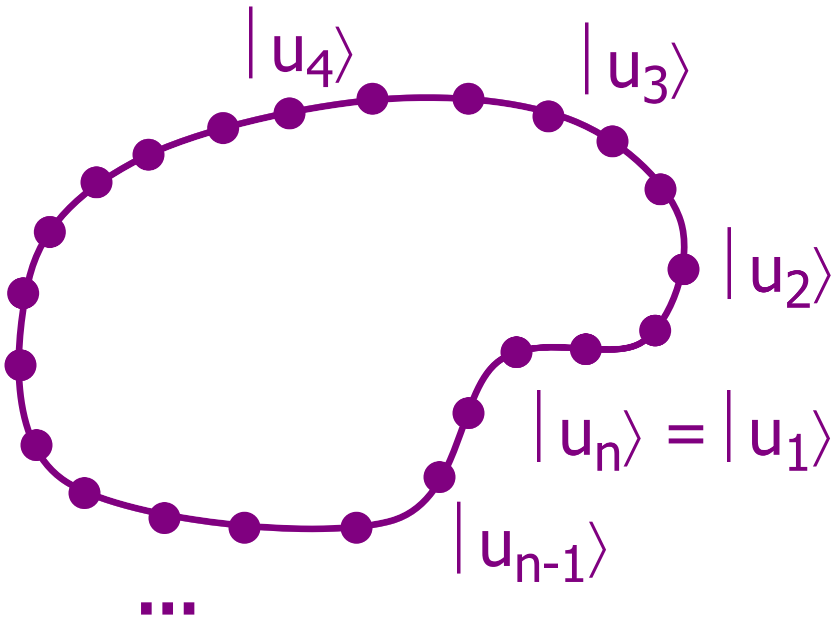
NSF DMR-1408838

QMS23, August 21-25, 2023

# Outline

- Berry phases and curvatures
- Anomalous Hall (AH) effect
- Quantum anomalous Hall (QAH) effect
- Nonlinear Hall effect
- Semiclassical viewpoint
- Properties of Bloch electrons
- Summary

# Berry phases

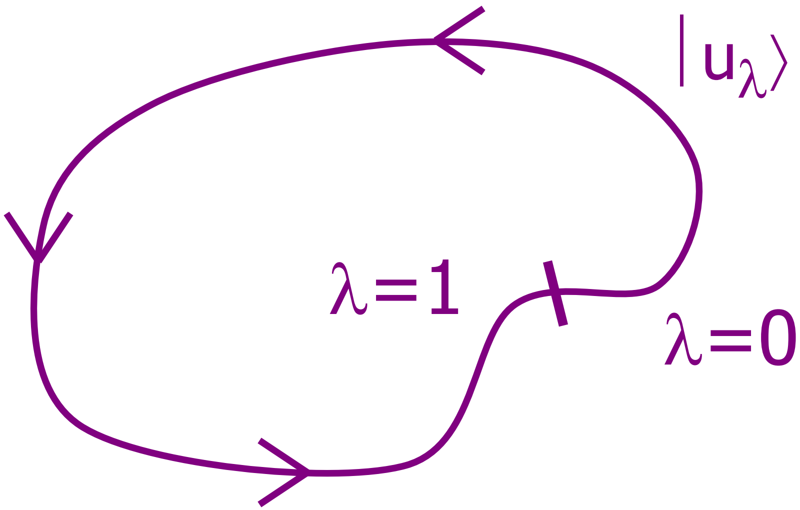



Now take limit that density of points $\rightarrow\infty$

$$\phi = -\mathrm{Im}\,\ln\left[\,\langle u_1|u_2\rangle\,\langle u_2|u_3\rangle \ldots \langle u_{n-1}|u_n\rangle\,\right]$$

Check: $|\widetilde{u}_2\rangle = e^{i\beta}\,|u_2\rangle$ has no effect.

# Berry phases




$$\boxed{\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \frac{du_\lambda}{d\lambda} \rangle}$$

$$\langle u_\lambda | \frac{d}{d\lambda} | u_\lambda \rangle$$

Gauge freedom

$$|\tilde{u}_\lambda\rangle = e^{i\beta(\lambda)} \, |u_\lambda\rangle$$

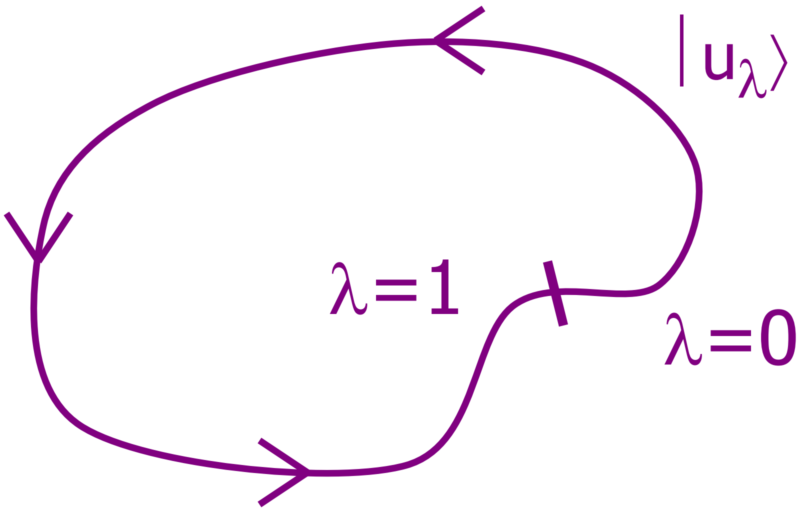
Continuity requires

$$e^{i\beta(1)} = e^{i\beta(0)}$$

Effect on Berry phase

$$\begin{aligned}\tilde{\phi} &= \phi + \int_0^1 d\lambda \, \frac{d\beta}{d\lambda} \\ &= \phi + [\beta(1) - \beta(0)] \\ &= \phi + 2\pi \ \times \ \text{integer}\end{aligned}$$

# Berry phases




$\phi$ is well-defined modulo $2\pi$

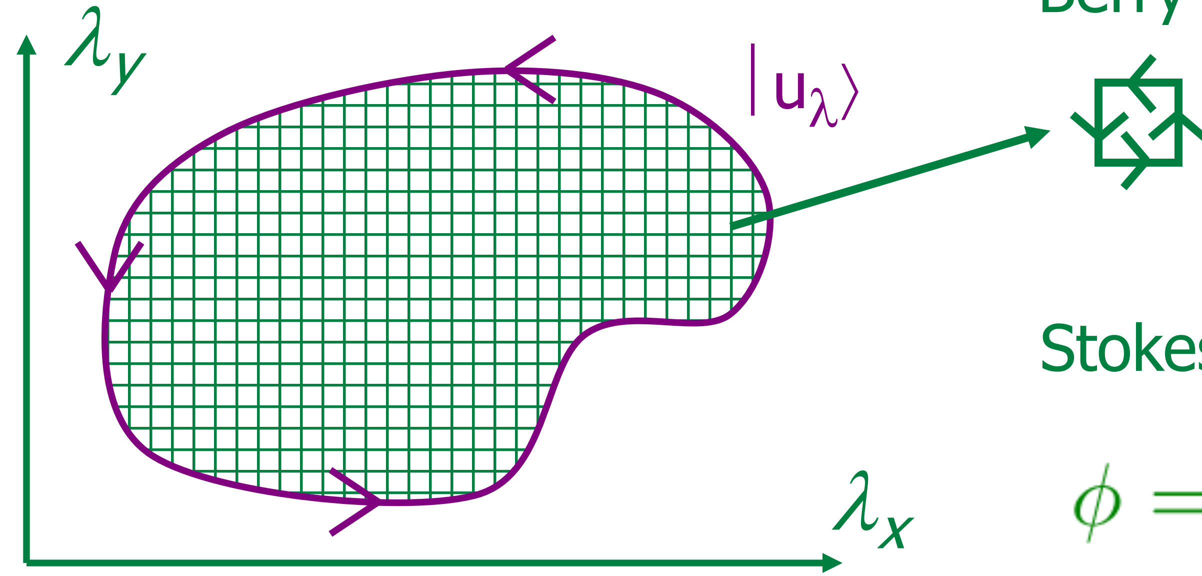
$\Rightarrow$ $\phi$ is a phase

$$\boxed{\phi = -\mathrm{Im} \oint d\lambda \, \langle u_\lambda | \tfrac{d}{d\lambda} | u_\lambda \rangle}$$

$$\phi = \oint d\lambda \, A(\lambda) \quad , \qquad \boxed{A(\lambda) = \langle u_\lambda | i \tfrac{d}{d\lambda} | u_\lambda \rangle}$$

"Berry connection"
or
"Berry potential"

# Berry curvature




Berry phase per unit area

$$\Omega = \Delta\phi / \Delta A_\lambda$$

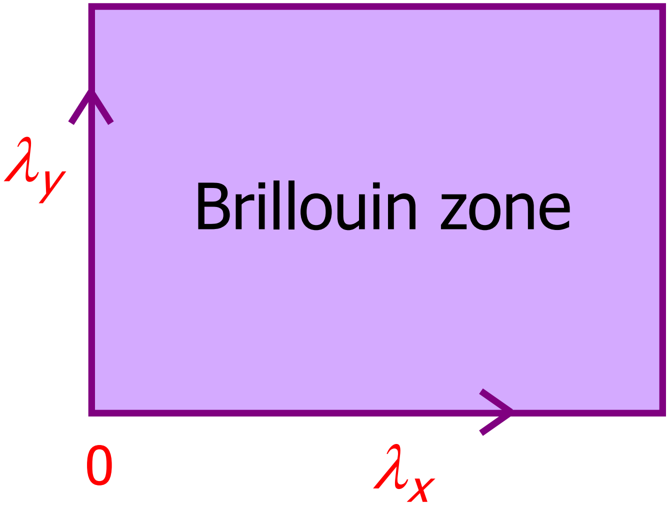
Stokes theorem

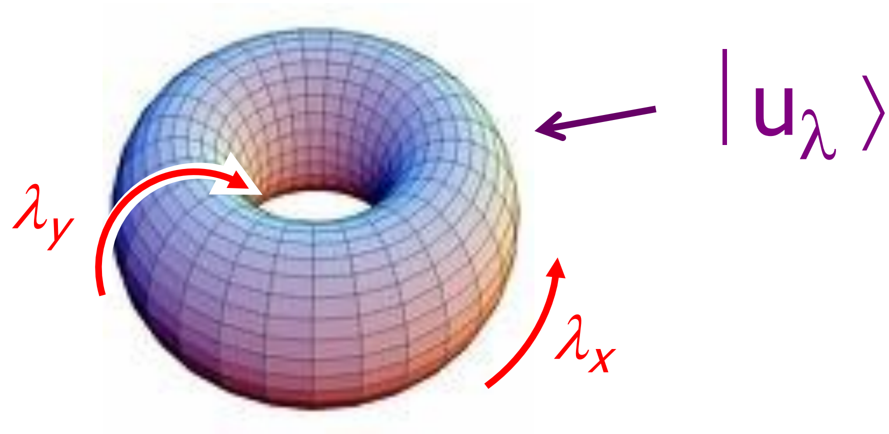
$$\phi = \int \Omega(\lambda)\; dS_\lambda$$

$$\phi = -\mathrm{Im} \oint \langle u_\lambda | \boldsymbol{\nabla}_\lambda | u_\lambda \rangle \cdot d\boldsymbol{\lambda}$$

$$\Omega = -2\,\mathrm{Im} \left\langle \frac{du}{d\lambda_x} \middle| \frac{du}{d\lambda_y} \right\rangle$$

# Chern theorem



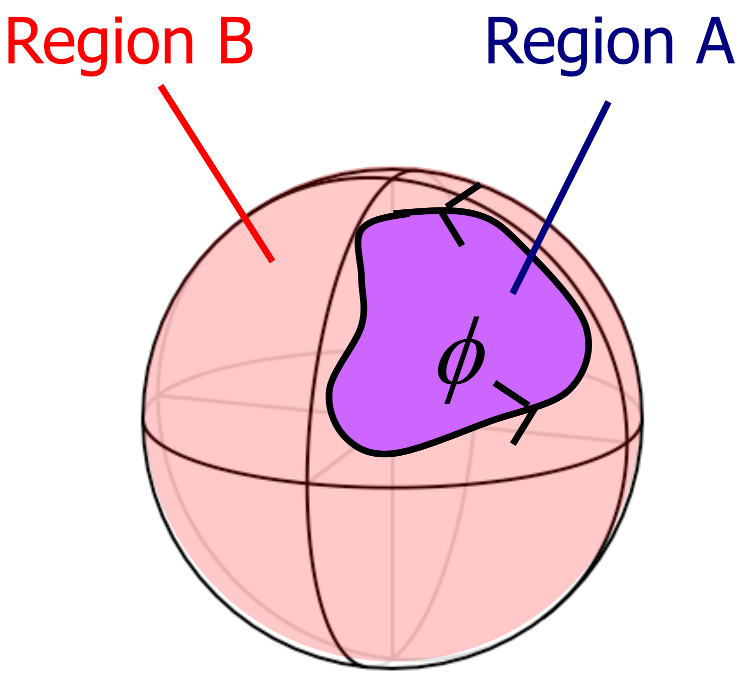




$$\boxed{\oint \Omega(\lambda)\, dS_\lambda = 2\pi\, C}$$

Berry curvature

Chern number

# Chern theorem




Stokes applied to A:

$$\phi = \int_A \Omega(\lambda)\, dS_\lambda \mod 2\pi$$

Stokes applied to B:

$$\phi = -\int_B \Omega(\lambda)\, dS_\lambda \mod 2\pi$$

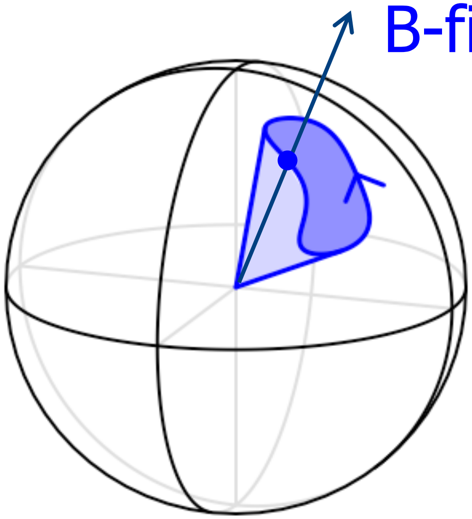
Subtract:

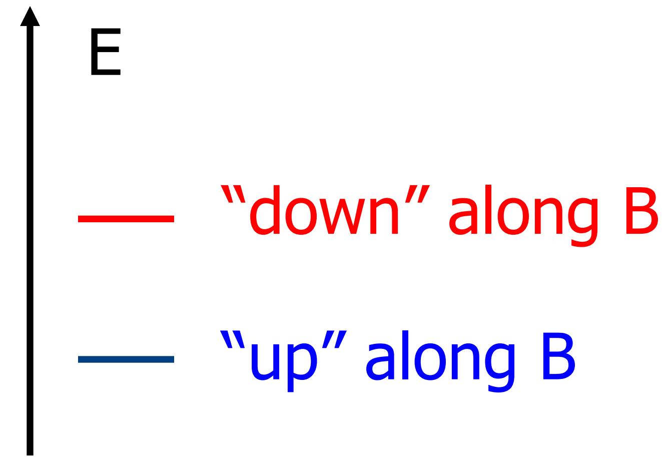
$$0 = \oint \Omega(\lambda)\, dS_\lambda \mod 2\pi$$

Chern theorem: $\oint \Omega(\lambda)\, dS_\lambda = 2\pi\, C$

# Example: Spinor on Bloch sphere

Famous example: Spinor in magnetic field




$$\Omega = \frac{d(\text{Berry phase})}{d(\text{solid angle})} = \frac{1}{2}$$

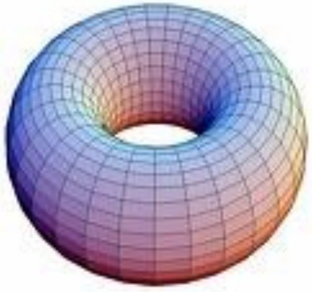
$$C = \frac{1}{2\pi}\oint \Omega \, d(\text{solid angle}) = \frac{1}{2\pi}(\Omega \cdot 4\pi) = 1$$

# 2D crystalline insulators

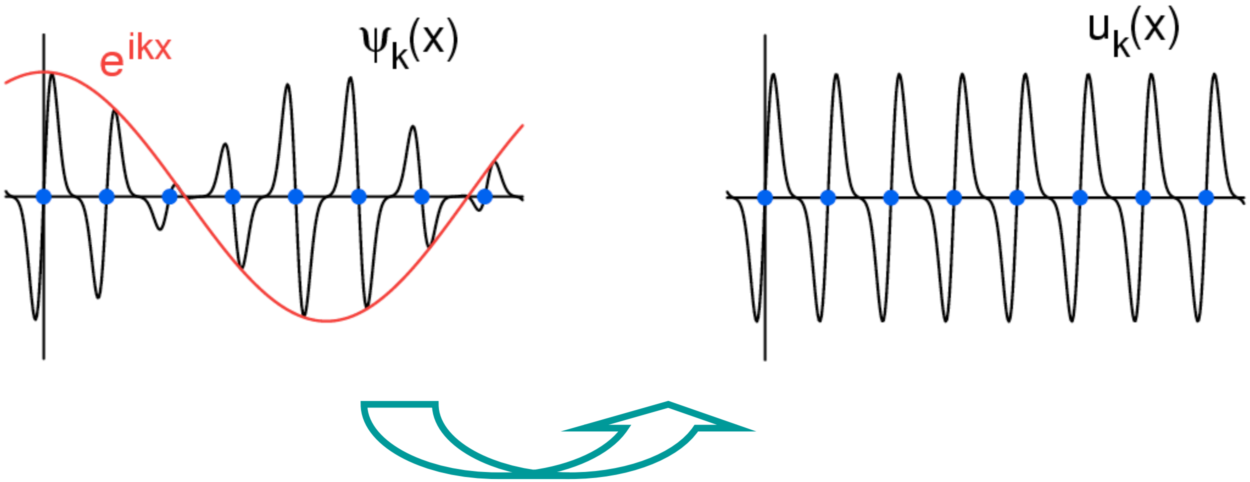
$$(\lambda_x, \lambda_y) \Rightarrow (k_x, k_y)$$

General Parametric Hamiltonian

2D insulator on k-space torus



# Cell-periodic Bloch functions




Define the cell-periodic Bloch function $u_k(x)$:

$$u_k(x) = e^{-ikx}\psi_k(x)$$

These obey the same periodic boundary conditions, independent of *k.*

Thus $du_k / dk$ is well defined, while $d\psi_k / dk$ is not.

# Berryology of the 3D Brillouin zone

Component notation

Berry connection $A_a(\mathbf{k}) = \langle u_\mathbf{k} | i\partial_a | u_\mathbf{k}\rangle$ $\qquad \partial_a = \partial/\partial k_a$

Berry curvature (pseudovector) $\Omega_a(\mathbf{k}) = \epsilon_{abc}\, \partial_b\, A_c(\mathbf{k})$ $\qquad \Omega_{ab} = \epsilon_{abc}\Omega_c$

Berry curvature (tensor) $\Omega_{ab}(\mathbf{k}) = -2\mathrm{Im}\, \langle \partial_a u_\mathbf{k} | \partial_b u_\mathbf{k}\rangle$

Vector notation

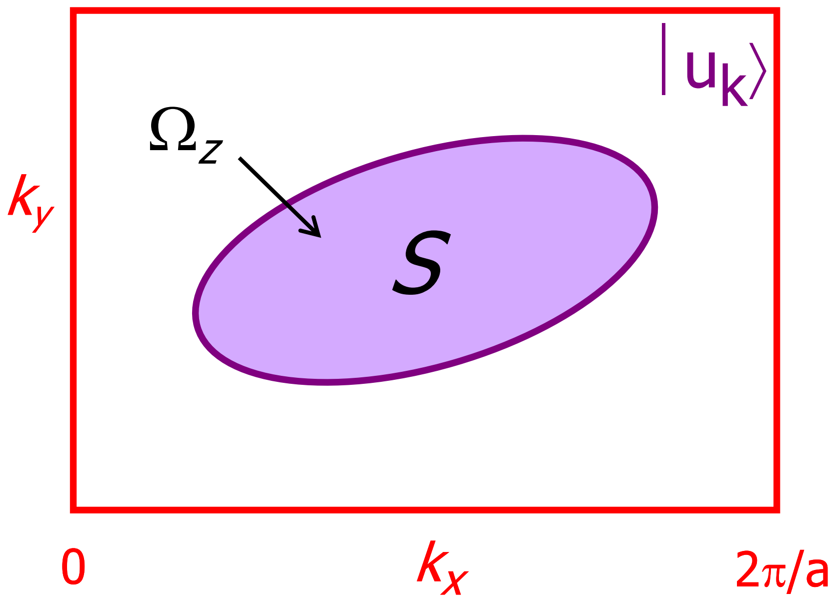
$$\mathbf{A}(\mathbf{k}) = \langle u_\mathbf{k} | i\boldsymbol{\nabla}_\mathbf{k} | u_\mathbf{k}\rangle$$

$$\boldsymbol{\Omega}(\mathbf{k}) = \boldsymbol{\nabla}_\mathbf{k} \times \mathbf{A}(\mathbf{k})$$

Compare $\mathbf{B}(\mathbf{r}) = \boldsymbol{\nabla}_\mathbf{r} \times \mathbf{A}^{\mathrm{EM}}(\mathbf{r})$

$$\boldsymbol{\Omega}(\mathbf{k}) = -2\mathrm{Im}\, \langle \boldsymbol{\nabla}_\mathbf{k} u_\mathbf{k} | \times | \boldsymbol{\nabla}_\mathbf{k} u_\mathbf{k}\rangle$$

# Meaning of Berry curvature in a FM metal



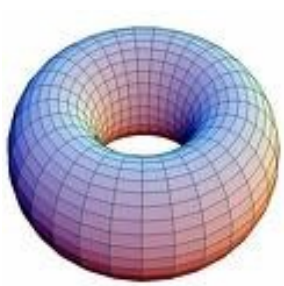

$$\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x} \middle| \frac{du}{dk_y} \right\rangle$$

$$\sigma_{yx} = \frac{e^2}{h}\,\frac{1}{2\pi}\int_S \Omega_z(\mathbf{k})\, d^2k$$

Fermi sea

Anomalous Hall conductivity !

**(Intrinsic part !)**



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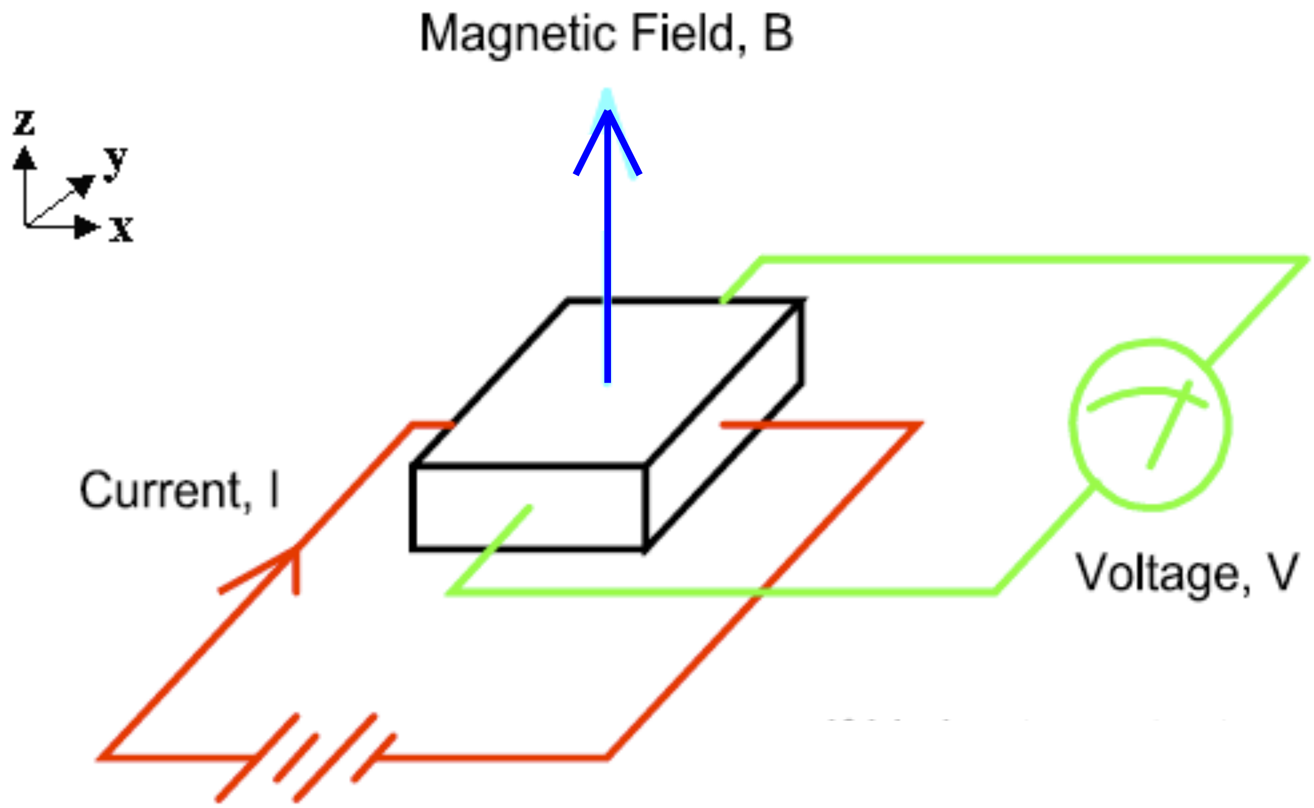
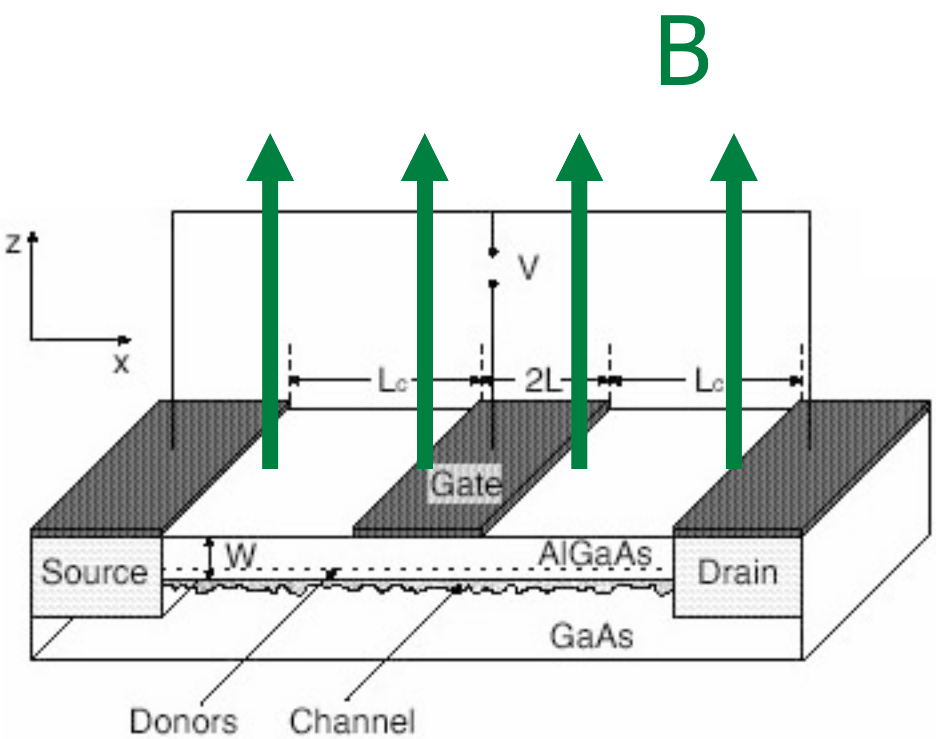
# Ordinary Hall conductivity

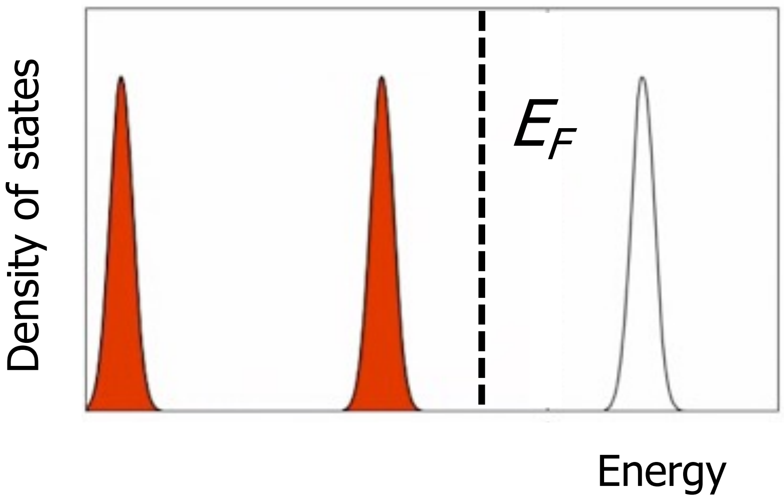


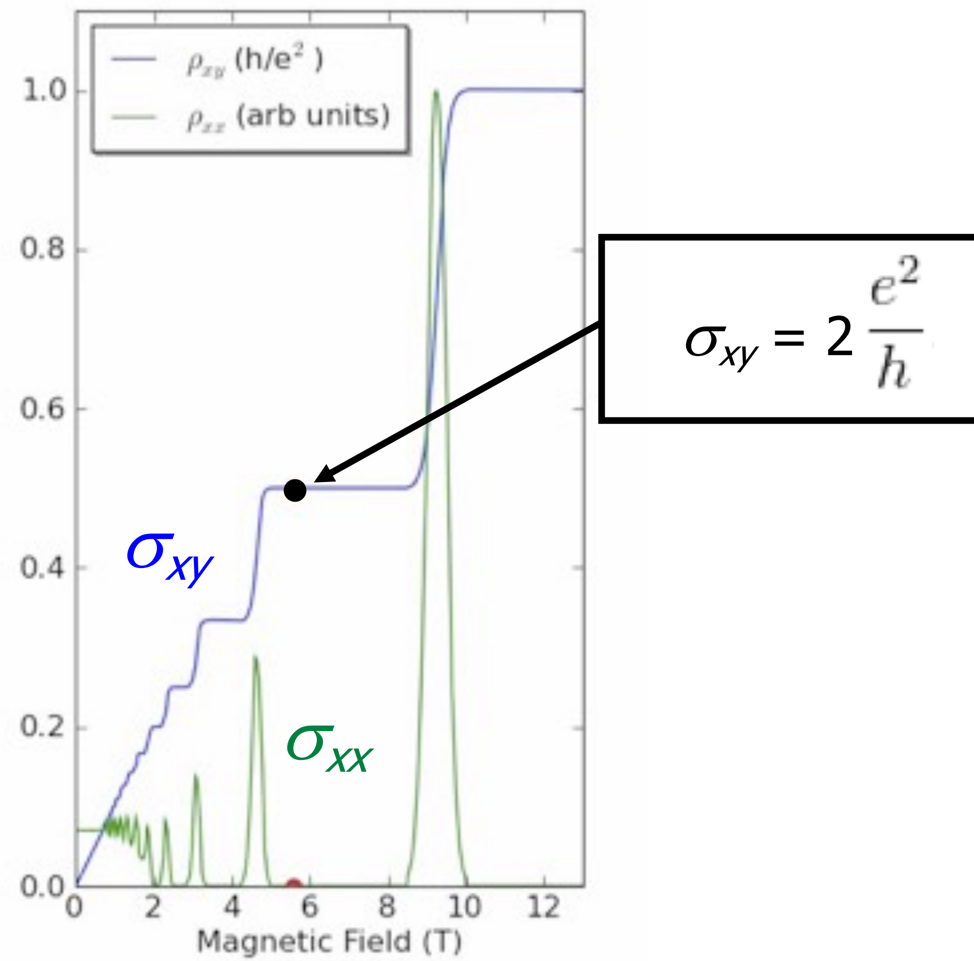

Measure $\sigma_{xy}$ in presence of *B*-field

# Quantum Hall effect



# Quantum Hall effect

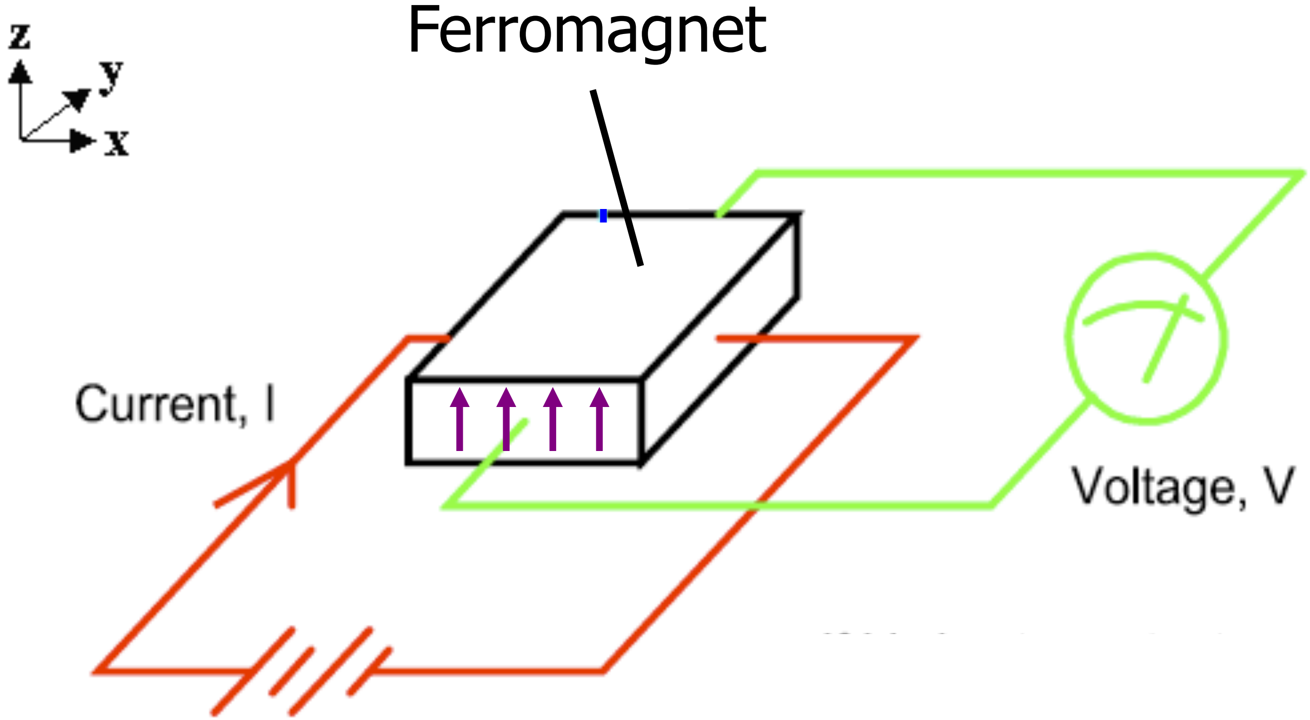


# Hall effects: The big picture

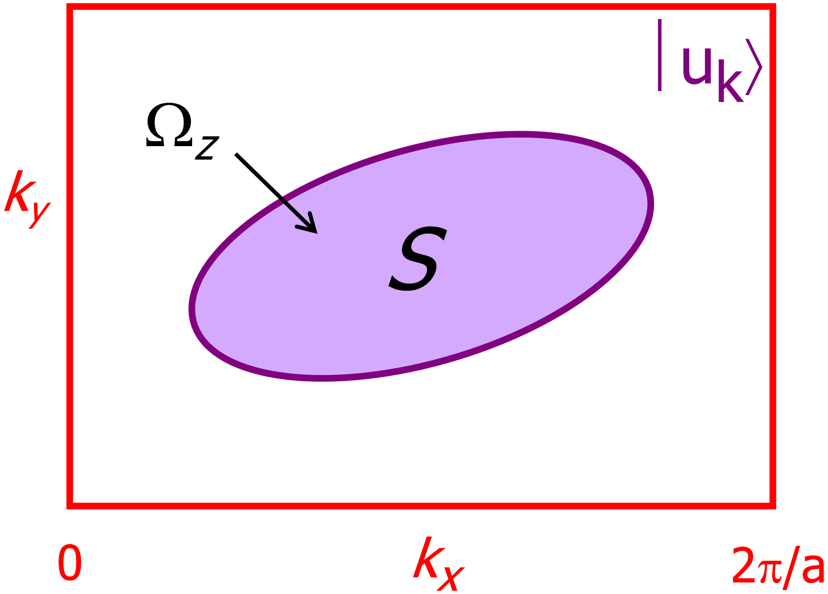
| | Induced by B-field | Ferromagnetic sample |
|---|---|---|
| Metal | Ordinary Hall (1879) | |
| Topological insulator | Quantum Hall (1980) | |

# Anomalous Hall conductivity (AHC)




Measure $\sigma_{xy}$ in *absence* of *B*-field

# Berry curvature in a FM metal



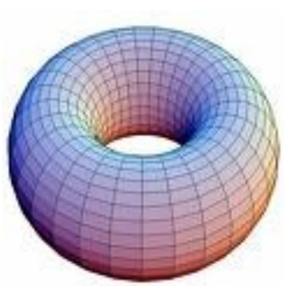

$$\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x} \middle| \frac{du}{dk_y} \right\rangle$$

$$\sigma_{yx} = \frac{e^2}{h}\frac{1}{2\pi}\int_S \Omega_z(\mathbf{k})\, d^2k$$

Fermi sea

Anomalous Hall conductivity !

**(Intrinsic part !)**



# Karplus-Luttinger intrinsic AHC

**Patrick Bruno**
*Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany*

TH–2007–20

From Kubo's linear response theory, the conductivity tensor for independent electrons is given by Luttinger (1969)

$$\sigma_{ij} = \frac{ie^2\hbar}{\Omega}\lim_{s\to 0^+} \times \left\langle \sum_{n,m} \frac{f(\varepsilon_n) - f(\varepsilon_m)}{\varepsilon_m - \varepsilon_n} \frac{\langle n| v_j |m\rangle \langle m| v_i |n\rangle}{\varepsilon_n - \varepsilon_m + is} \right\rangle_c \quad (76)$$

$$\langle u_{m\mathbf{k}}|\partial_{\mathbf{k}}|u_{n\mathbf{k}}\rangle = \hbar\frac{\langle u_{n\mathbf{k}}|\mathbf{v}|u_{m\mathbf{k}}\rangle}{\epsilon_{n\mathbf{k}} - \epsilon_{m\mathbf{k}}}$$

$$\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x} \middle| \frac{du}{dk_y} \right\rangle$$

Modern view:

$$\boxed{\sigma_{ij} = -\frac{e^2}{h}\int_{\mathrm{BZ}} \frac{d^2k}{(2\pi)^2} \sum_n f(\epsilon_{n\mathbf{k}})\,\Omega_{n\mathbf{k},ij}}$$

# Symmetries of Berry curvature

## Symmetries

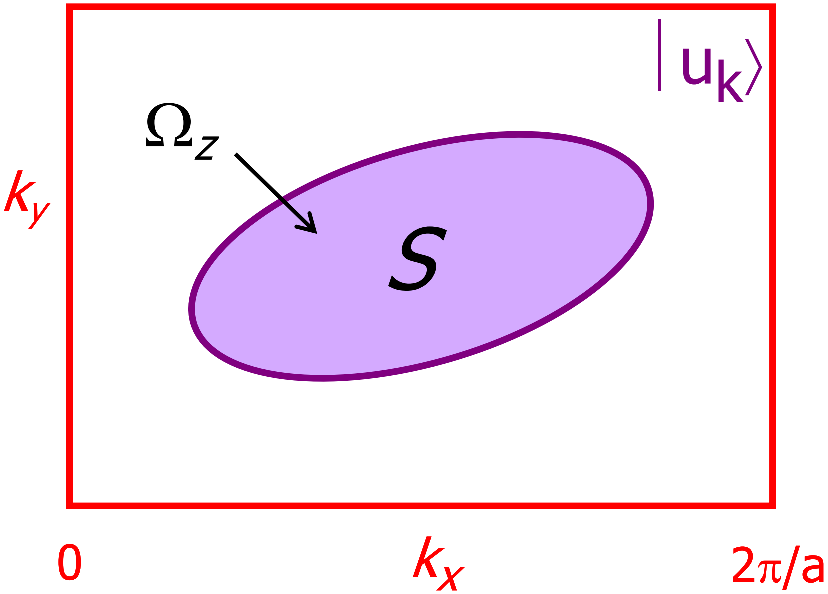
- Inversion: $\Omega(\mathbf{k}) = \Omega(-\mathbf{k})$
- TR: $\Omega(\mathbf{k}) = -\Omega(-\mathbf{k})$

## Consequences

- Nonmag. centrosymm.: $\Omega(\mathbf{k}) = 0$
- Nonmag. acentric: $\int \Omega(\mathbf{k})\, d^3k = 0$
- FM: $\int \Omega(\mathbf{k})\, d^3k \neq 0$

over Fermi sea (metal)
or
BZ (insulator)

# Berry curvature in a FM metal



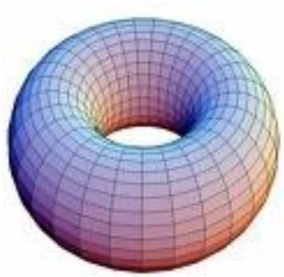

$$\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x} \middle| \frac{du}{dk_y} \right\rangle$$

$$\sigma_{yx} = \frac{e^2}{h}\frac{1}{2\pi}\int_S \Omega_z(\mathbf{k})\, d^2k$$

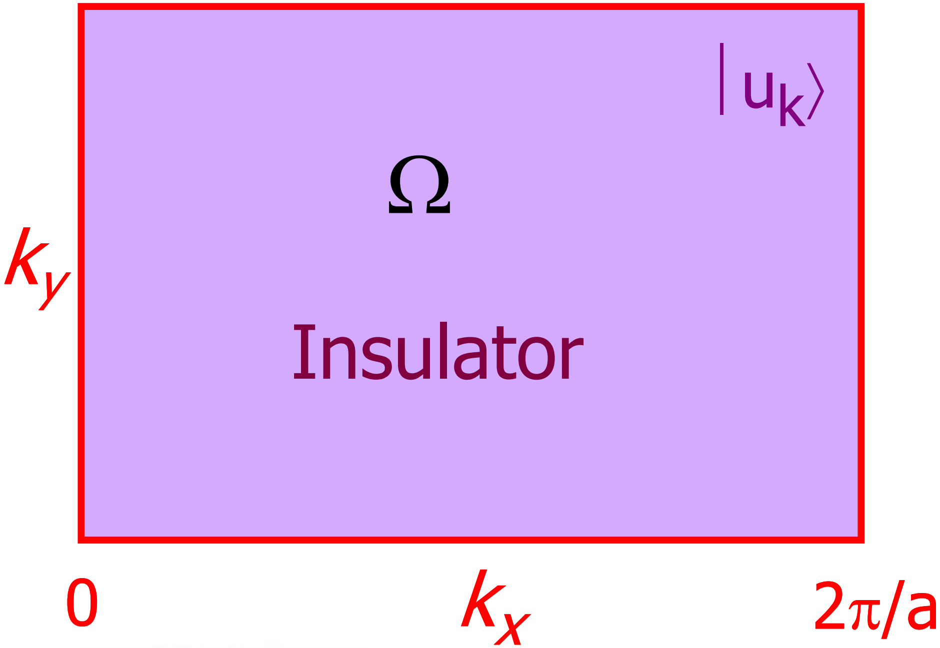
Fermi sea

Anomalous Hall conductivity !

**(Intrinsic part !)**

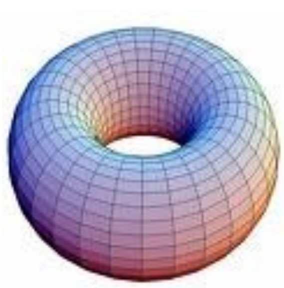


# Berry curvature in a FM insulator




$$\Omega_z(\mathbf{k}) = -2\mathrm{Im}\left\langle \frac{du}{dk_x} \middle| \frac{du}{dk_y} \right\rangle$$

$$\sigma_{yx} = \frac{e^2}{h}\,\frac{1}{2\pi}\underbrace{\int_{\mathrm{BZ}} \Omega_z(\mathbf{k})\, d^2k}_{2\pi C}$$



$$\sigma_{yx} = \frac{e^2}{h} C$$

Chern number (integer)

Quantum anomalous Hall (QAH) insulator

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# Hall effects: The big picture

| | Induced by B-field | Ferromagnetic sample |
|---|---|---|
| Metal | Ordinary Hall (1879) | Anomalous Hall (1881) |
| Topological insulator | Quantum Hall (1980) | Quantum Anomalous Hall (2013) |

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- **Quantum anomalous Hall (QAH) effect**
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# Proof of principle: QAH insulators

VOLUME 61, NUMBER 18 PHYSICAL REVIEW LETTERS 31 OCTOBER 1988

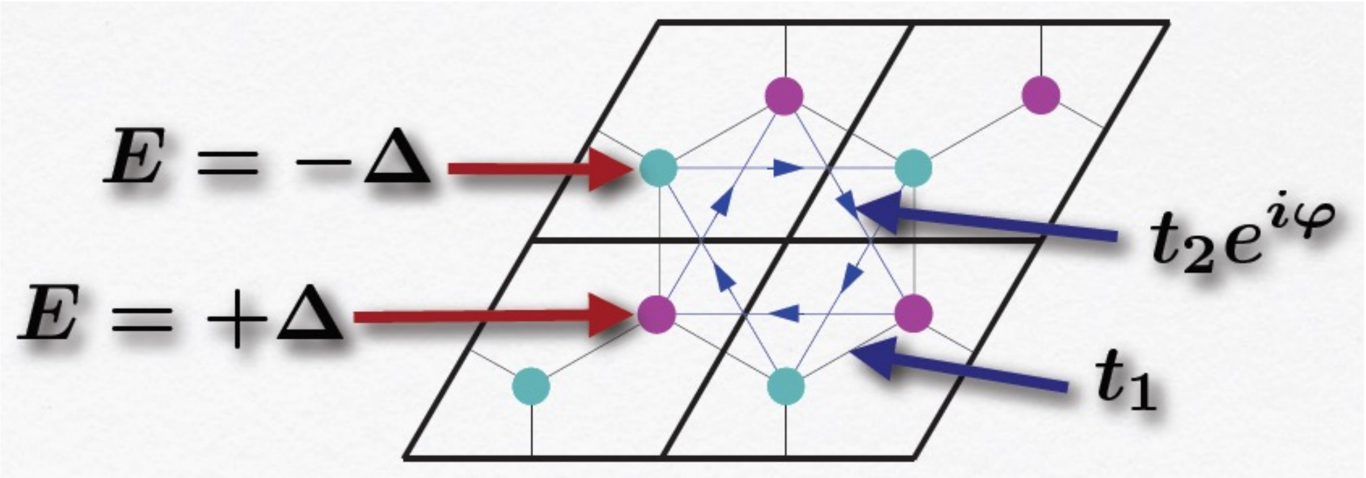
**Model for a Quantum Hall Effect without Landau Levels: Condensed-Matter Realization of the "Parity Anomaly"**

F. D. M. Haldane

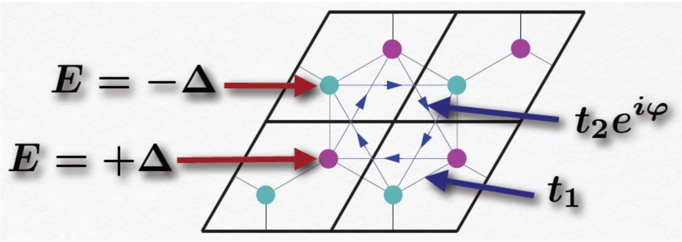
*Department of Physics, University of California, San Diego, La Jolla, California 92093*

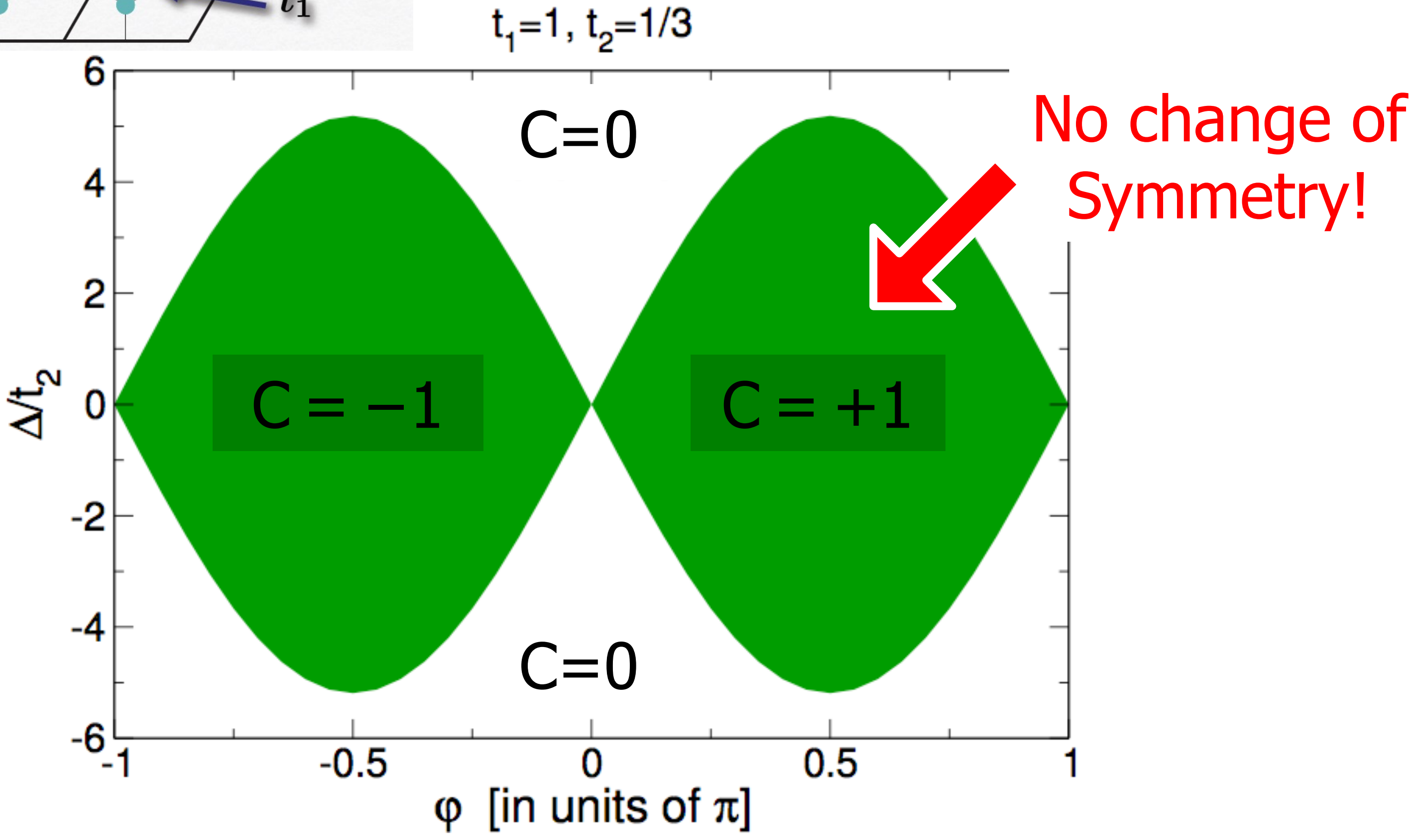
(Received 16 September 1987)

A two-dimensional condensed-matter lattice model is presented which exhibits a nonzero quantization of the Hall conductance $\sigma^{xy}$ in the *absence* of an external magnetic field. Massless fermions *without spectral doubling* occur at critical values of the model parameters, and exhibit the so-called "parity anomaly" of (2+1)-dimensional field theories.



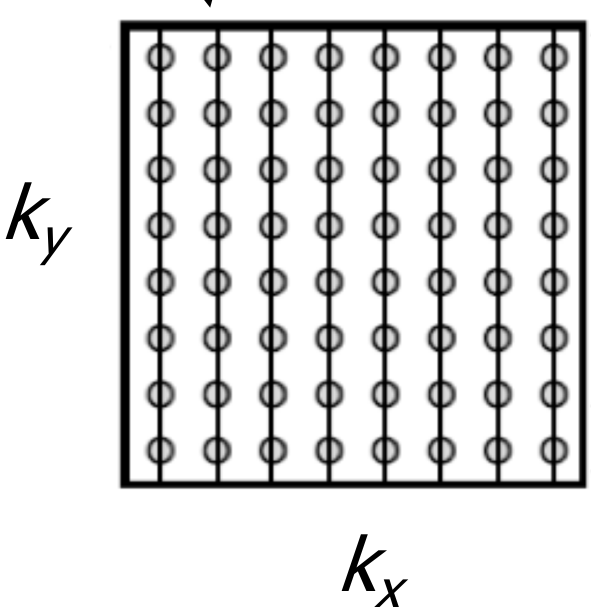
# Phase diagram of Haldane model

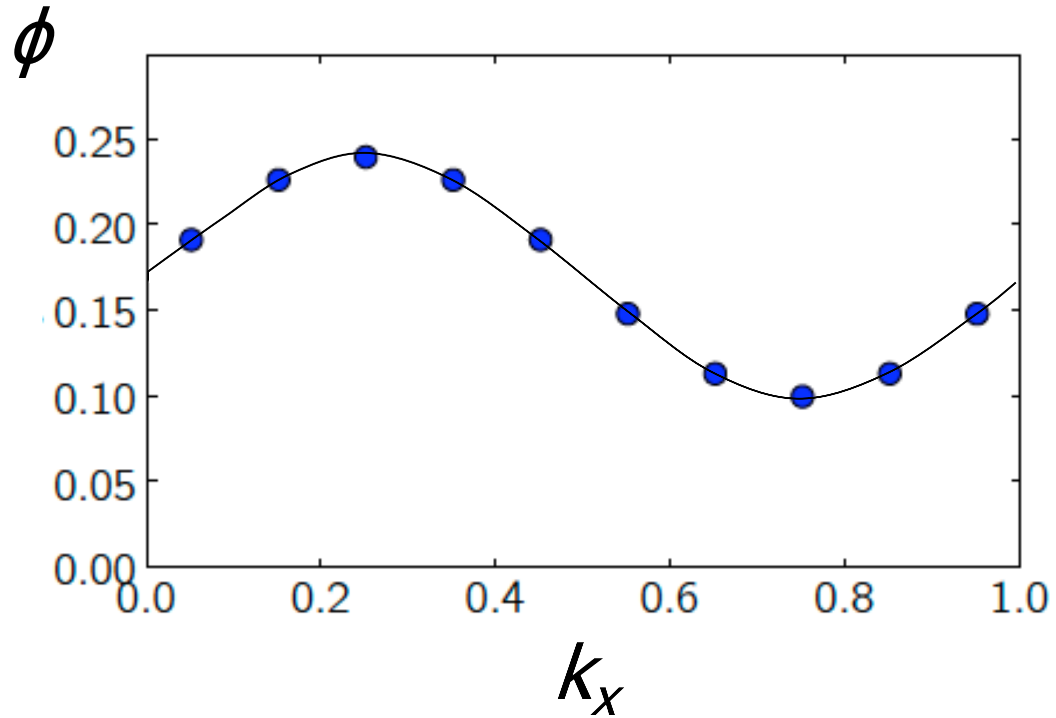


# String Berry phases for normal band

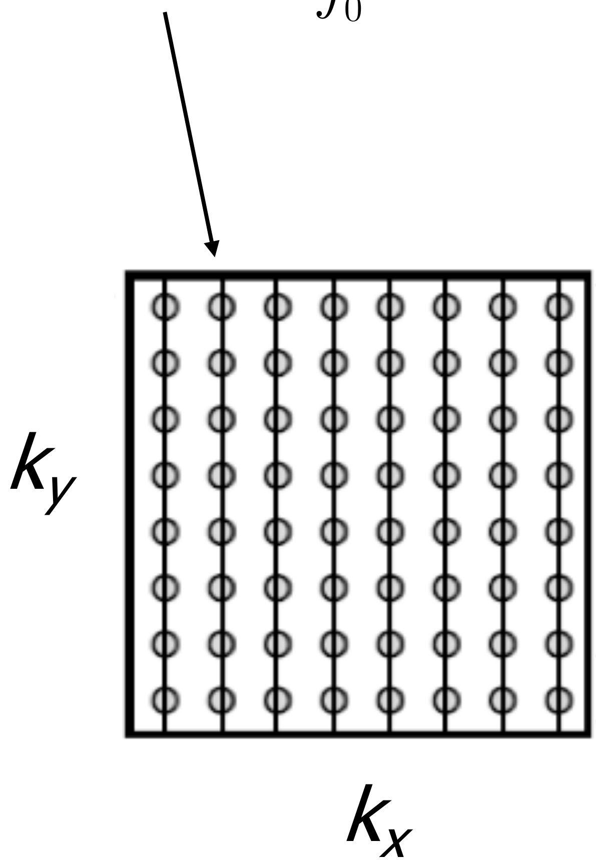
$$\phi_y(k_x) = \int_0^{2\pi/b} dk_y \; A_y(k_x, k_y)$$

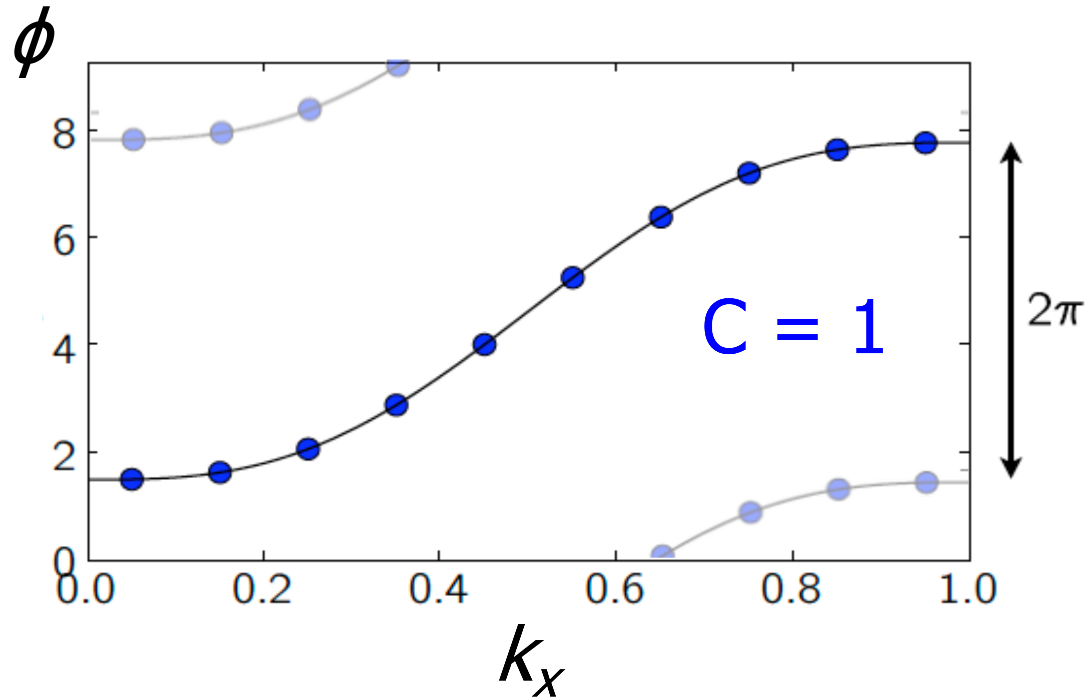


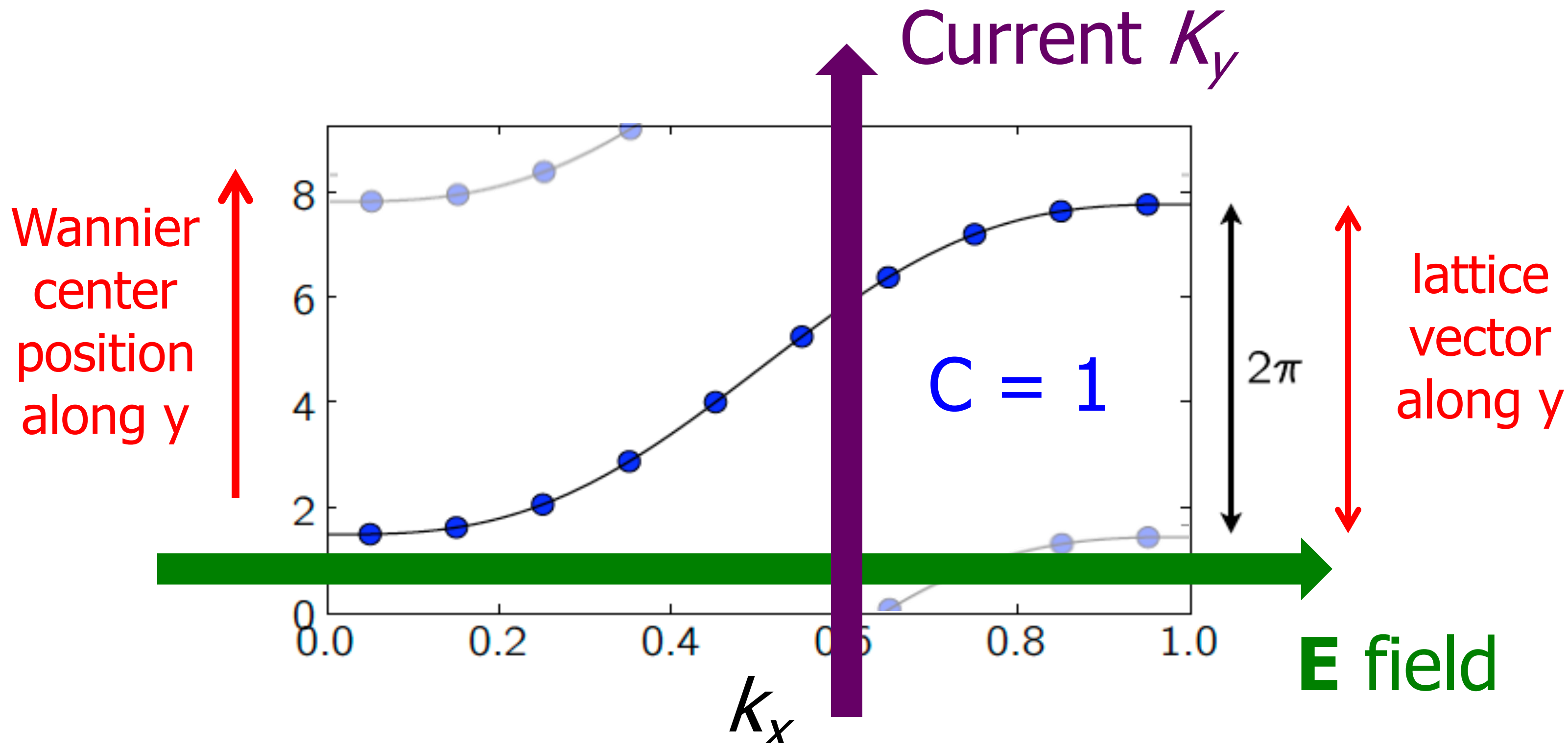
# String Berry phases in QAH band

$$\phi_y(k_x) = \int_0^{2\pi/b} dk_y \; A_y(k_x, k_y)$$



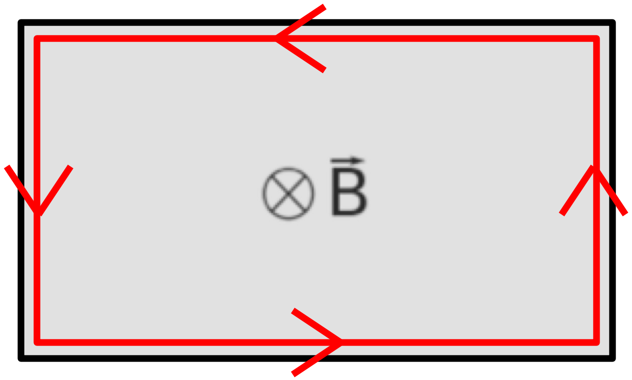
# Physical relation to anomalous Hall



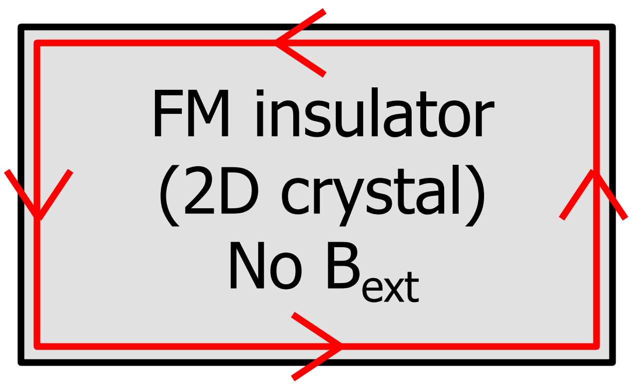

$$\sigma_{yx} = \frac{e^2}{h} C$$

# Quantum Hall Edge Channels

- Quantum Hall:




- Quantum anomalous Hall:

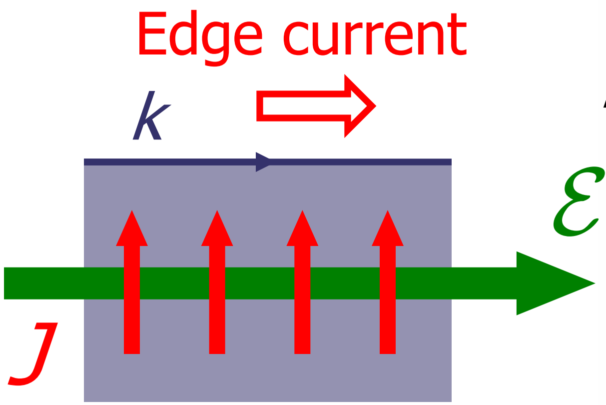


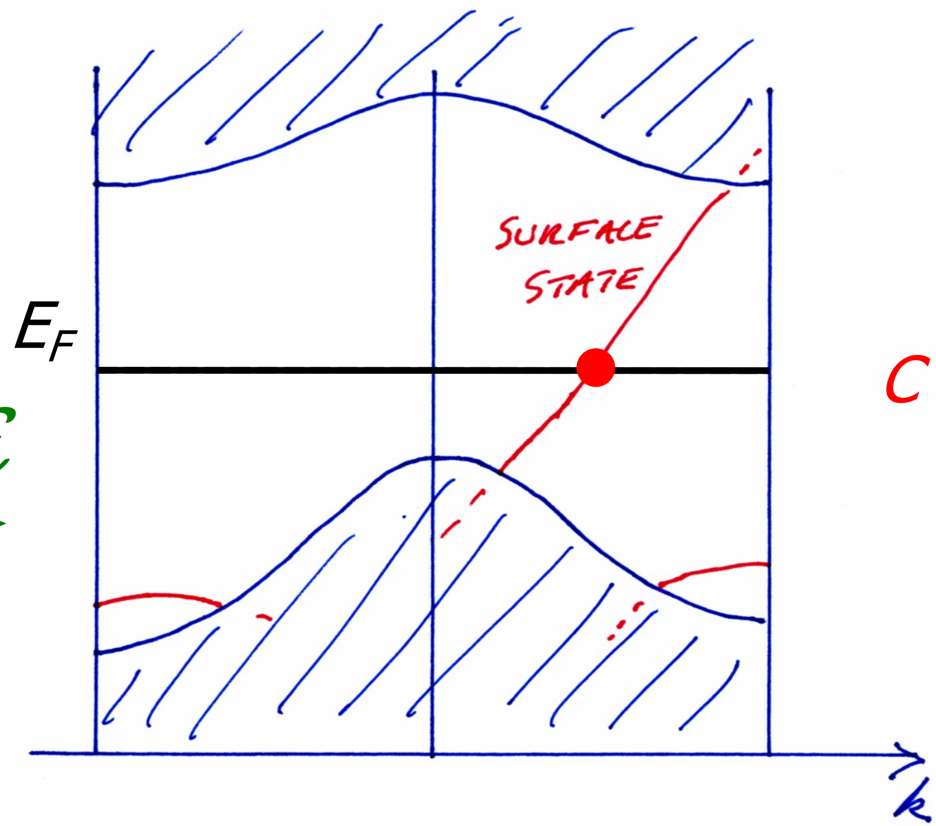

Chiral edge channels

$\sigma_{yx} = e^2/h$

exactly !

# Edge states: 2D QAH insulator




$C = +1$

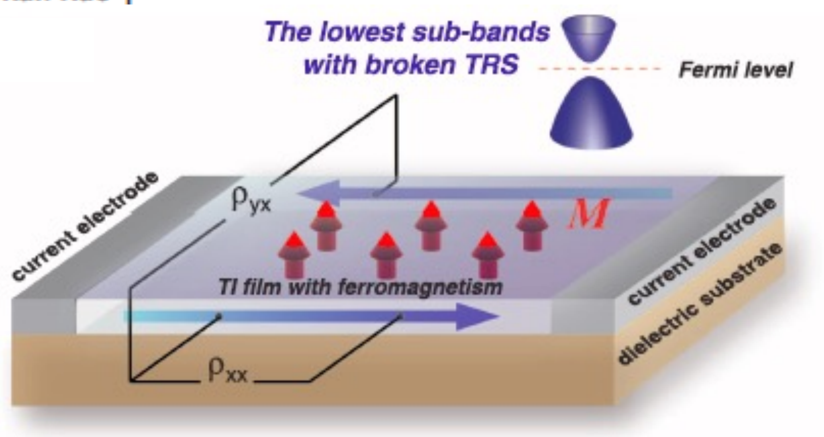
Conservation of charge $\Rightarrow$ chiral surface state

# Magnetic doping: Claim for QAH

www.sciencemag.org SCIENCE VOL 340 12 APRIL 2013

## Experimental Observation of the Quantum Anomalous Hall Effect in a Magnetic Topological Insulator

Cui-Zu Chang,[1,2*] Jinsong Zhang,[1*] Xiao Feng,[1,2*] Jie Shen,[2*] Zuocheng Zhang,[1] Minghua Guo,[1] Kang Li,[2] Yunbo Ou,[2] Pang Wei,[2] Li-Li Wang,[2] Zhong-Qing Ji,[2] Yang Feng,[1] Shuaihua Ji,[1] Xi Chen,[1] Jinfeng Jia,[1] Xi Dai,[2] Zhong Fang,[2] Shou-Cheng Zhang,[3] Ke He,[2†] Yayu Wang,[1†] Li Lu,[2] Xu-Cun Ma,[2] Qi-Kun Xue[1†]




Observed below ~1K

# Discovery of QAH (2013)

www.sciencemag.org SCIENCE VOL 340 12 APRIL 2013

**Experimental Observation of the Quantum Anomalous Hall Effect in a Magnetic Topological Insulator**

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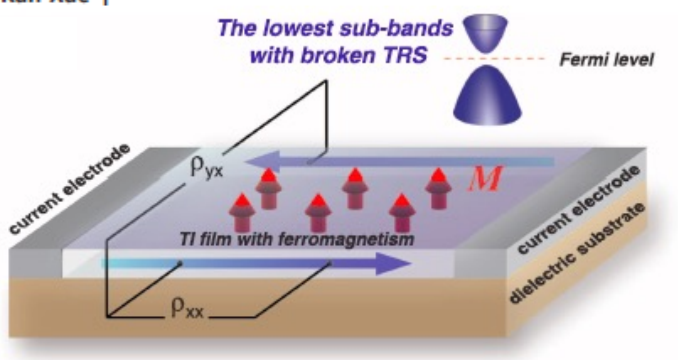
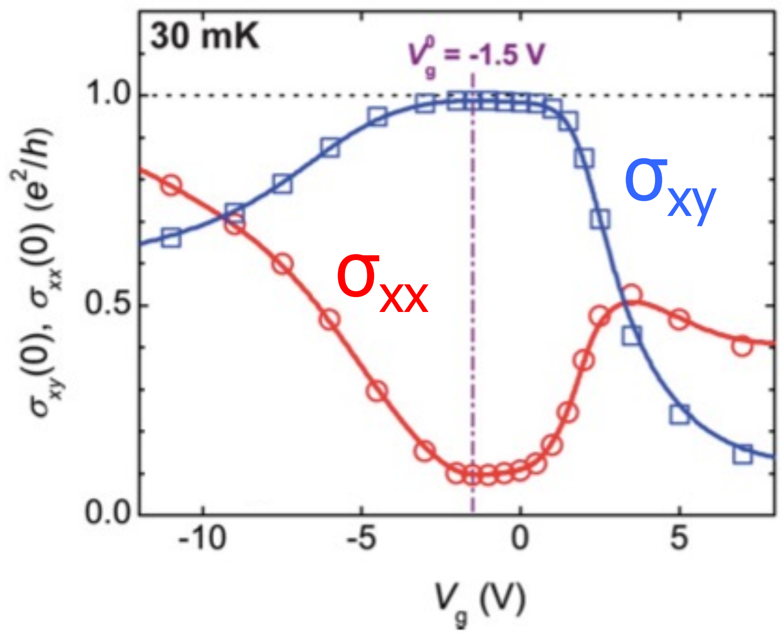



Cr-doped $(Bi,Sb)_2Te_3$ films




98% of $e^2/h$ at 30mK

# Higher T with V doping

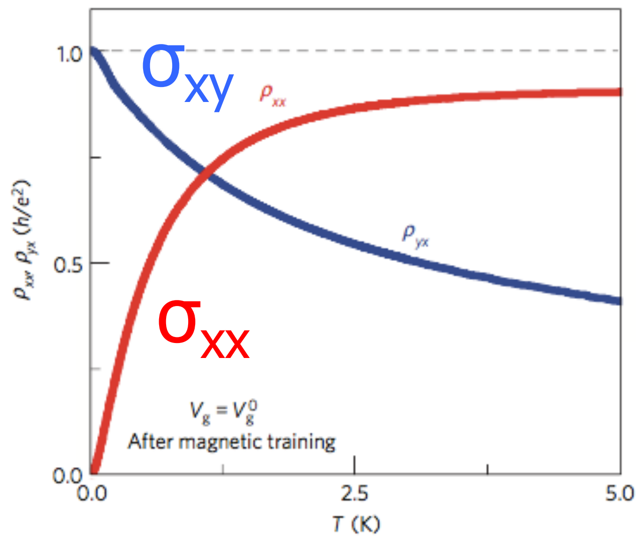
nature materials

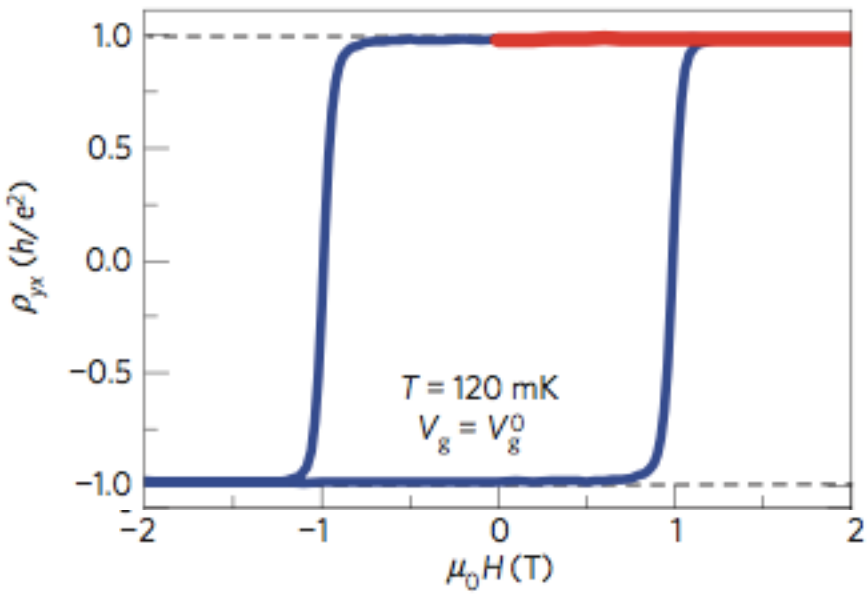
March 2015

**High-precision realization of robust quantum anomalous Hall state in a hard ferromagnetic topological insulator**

Cui-Zu Chang[1]*, Weiwei Zhao[2]*, Duk Y. Kim[2], Haijun Zhang[3], Badih A. Assaf[4], Don Heiman[4], Shou-Cheng Zhang[3], Chaoxing Liu[2], Moses H. W. Chan[2] and Jagadeesh S. Moodera[1,5]*

V-doped $(Bi,Sb)_2Te_3$ films




97% of $e^2/h$ at 200mK

99.98% of $e^2/h$ at 25mK

# Hall effects: The big picture

| | Induced by B-field | Ferromagnetic sample |
|---|---|---|
| Metal | Ordinary Hall (1879) | Anomalous Hall (1881) |
| Topological insulator | Quantum Hall (1980) | Quantum Anomalous Hall (2013) |

# Outline

- Berry phases and curvatures
- Anomalous Hall (AH) effect
- Quantum anomalous Hall (QAH) effect
- **Nonlinear Hall effect**
- Semiclassical viewpoint
- Properties of Bloch electrons
- Summary

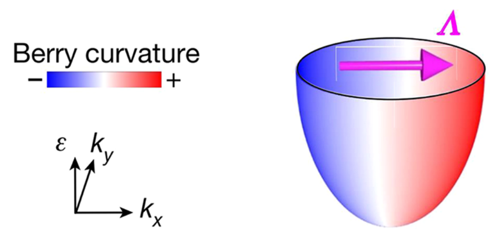
# Nonlinear Hall effect

PRL **115,** 216806 (2015) PHYSICAL REVIEW LETTERS week ending 20 NOVEMBER 2015

**Quantum Nonlinear Hall Effect Induced by Berry Curvature Dipole in Time-Reversal Invariant Materials**

Inti Sodemann and Liang Fu

- Consider nonmagnetic but acentric conductor ("polar metal")
- $\Omega(\mathbf{k}) = -\Omega(-\mathbf{k})$ so that $\int_{BZ} \Omega(\mathbf{k}) f(\mathbf{k})\, d^3k = 0$
- Apply $E$ and drive current $J \propto \tau E$
  - Fermi surface shifts $\propto \tau E$
  - Now $\int_{BZ} \Omega\, d^3k \neq 0$




Wang, Ye, Yu, and Liao, ACS Nano 14, 3755 (2020)

# Nonlinear Hall effect

$$j_a^0 = \chi_{\text{abc}} \mathcal{E}_b \mathcal{E}_c^*$$ (also $j_a^{2\omega} = \chi_{\text{abc}} \mathcal{E}_b \mathcal{E}_c$)

$$\chi_{\text{abc}} = \varepsilon_{\text{adc}} \frac{e^3 \tau}{2(1 + i\omega\tau)} \int_k (\partial_b f_0) \boldsymbol{\Omega}_d$$
$$= -\varepsilon_{adc} \frac{e^3 \tau}{2(1 + i\omega\tau)} \int_k f_0 (\partial_b \boldsymbol{\Omega}_d)$$

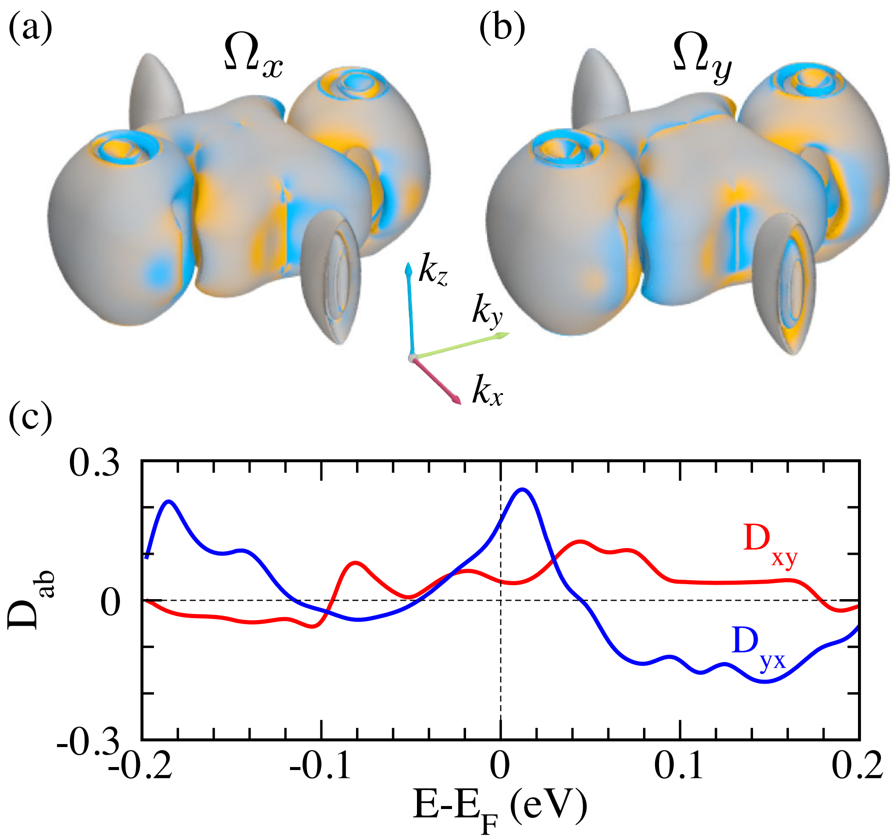
$$\boxed{D_{ab} = \int_k f_0 (\partial_a \Omega_b)}$$ "Berry curvature dipole moment" (BCDM)

# Nonlinear Hall effect

PHYSICAL REVIEW LETTERS **125,** 046402 (2020)

**Engineering Weyl Phases and Nonlinear Hall Effects in $T_d$-$MoTe_2$**

Sobhit Singh,* Jinwoong Kim, Karin M. Rabe, and David Vanderbilt
*Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854-8019, USA*



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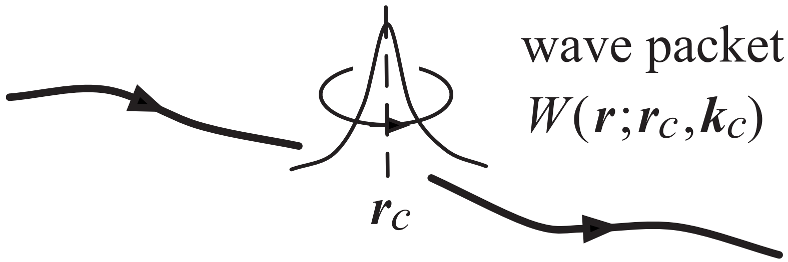
# Semiclassical wavepacket dynamics

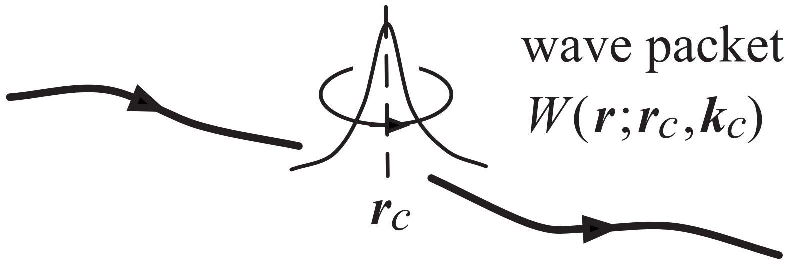



Dynamics of wave packet:

$$\dot{\boldsymbol{r}} = \frac{1}{\hbar}\frac{\partial \varepsilon_n(\boldsymbol{k})}{\partial \boldsymbol{k}}$$
$$\hbar\dot{\boldsymbol{k}} = -e\boldsymbol{E}(\boldsymbol{r}) - e\dot{\boldsymbol{r}} \times \boldsymbol{B}(\boldsymbol{r}),$$

This underlies the discussion of Boltzmann transport in most textbooks. But it is missing a term!

# Semiclassical wavepacket dynamics




Dynamics of wave packet:

$$\dot{\boldsymbol{r}} = \frac{1}{\hbar}\frac{\partial \varepsilon_n(\boldsymbol{k})}{\partial \boldsymbol{k}} \boxed{- \dot{\boldsymbol{k}} \times \boldsymbol{\Omega}_n(\boldsymbol{k}),}$$

$$\hbar\dot{\boldsymbol{k}} = -e\boldsymbol{E}(\boldsymbol{r}) - e\dot{\boldsymbol{r}} \times \boldsymbol{B}(\boldsymbol{r}),$$

Anomalous velocity term

Recall that Ω vanishes if inversion and TR are present.
Otherwise, must be included for anomalous Hall, etc!

Good review: D. Xiao, M.-C. Chang and Q. Niu, RMP 82, 1959 (2010) .

# Density of states renormalization

Wavepacket equations of motion:

$$\dot{\mathbf{r}} = \mathbf{v}_{\mathrm{g}} - \dot{\mathbf{k}} \times \boldsymbol{\Omega}\,,$$

$$\dot{\mathbf{k}} = -\frac{e}{\hbar}\boldsymbol{\mathcal{E}} - \frac{e}{\hbar c}\,\dot{\mathbf{r}} \times \mathbf{B}\,,$$

Move all r-dot, k-dot terms to left side:

$$\left(1 + \frac{e}{\hbar c}\mathbf{B}\cdot\boldsymbol{\Omega}\right)\dot{\mathbf{r}} = \mathbf{v}_{\mathrm{g}} + \frac{e}{\hbar}\,\boldsymbol{\mathcal{E}} \times \boldsymbol{\Omega} + \frac{e}{\hbar c}\,(\mathbf{v}_{\mathrm{g}}\cdot\boldsymbol{\Omega})\,\mathbf{B}\,,$$

$$\left(1 + \frac{e}{\hbar c}\mathbf{B}\cdot\boldsymbol{\Omega}\right)\dot{\mathbf{k}} = -\frac{e}{\hbar}\boldsymbol{\mathcal{E}} - \frac{e}{\hbar c}\mathbf{v}_{\mathrm{g}} \times \mathbf{B} - \frac{e^2}{\hbar^2 c}\,(\boldsymbol{\mathcal{E}}\cdot\mathbf{B})\,\boldsymbol{\Omega}\,.$$

DOS in phase space = $(2\pi)^{-3}\left(1 + \frac{e}{\hbar c}\mathbf{B}\cdot\boldsymbol{\Omega}\right)$

Density of states

# Orbital moment

D. Xiao, J. Shi, and Q. Niu, PRL **95**, 137205 (2005).

Dynamics of wave packet:

$$\dot{\boldsymbol{r}} = \frac{1}{\hbar}\frac{\partial \varepsilon_n(\boldsymbol{k})}{\partial \boldsymbol{k}} \boxed{- \dot{\boldsymbol{k}} \times \boldsymbol{\Omega}_n(\boldsymbol{k}),}$$

Anomalous velocity term

$$\hbar\dot{\boldsymbol{k}} = -e\boldsymbol{E}(\boldsymbol{r}) - e\dot{\boldsymbol{r}} \times \boldsymbol{B}(\boldsymbol{r}),$$


Magnetic moment of wave packet:

$$\boxed{\mathbf{m}_{n\mathbf{k}} = \frac{e}{2\hbar c}\mathrm{Im}\,\langle \boldsymbol{\nabla}_{\mathbf{k}} u_{n\mathbf{k}}| \times (H_{\mathbf{k}} - E_{n\mathbf{k}})|\boldsymbol{\nabla}_{\mathbf{k}} u_{n\mathbf{k}}\rangle}$$

RUTGERS

# Properties of electron in state $\psi_{n\boldsymbol{k}}$

Quantities needed for transport, Fermi liquid theory, …
at each $\psi_{n\boldsymbol{k}}$ :

- Band energy $E$
- Spin moment $\boldsymbol{\mu}_{\text{spin}}$
- Orbital moment $\boldsymbol{\mu}_{\text{orb}}$
- Berry curvature $\boldsymbol{\Omega}$

Pseudovectors with same symmetry requirements

And we frequently also need $\boldsymbol{k}$ derivatives like

$\partial_{\boldsymbol{k}} E_{n\boldsymbol{k}}$ = hbar $\boldsymbol{v}_{\text{F}}$ for Fermi velocity

$\partial_{\boldsymbol{k}} \boldsymbol{\Omega}_{n\boldsymbol{k}}$ for BCDM

etc.

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Slides available at https://is.gd/inFID2

# EXTRA

# Physical meaning of Berry phases

$$\phi_y(k_x) = \int_0^{2\pi/b} dk_y \; A_y(k_x, k_y)$$