Topological Properties of Quantum States of Condensed Matter: some recent surprises.

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I. Berry phases, zero-field Hall effect, and "one-way light"

II. Anomalous and Spin Hall effect, Topological insulators

III. Non-abelian FQHE states

Hall effect in ferromagnetic metals:

$$E_x = \rho_{xy} J^y \qquad \rho_{xy} = R_0 B^z$$ isotropic (cubic) case

Hall effect in ferromagnetic metals with B parallel to a magnetization in the z-direction, and isotropy in the x-y plane:

$$\rho_{xy} = R_s M^z + R_0 B^z$$

The anomalous extra term is constant when H_z is large enough to eliminate domain structures.

What non-Lorentz force is providing the sideways deflection of the current? Is it intrinsic, or due to scattering of electrons by impurities or local non-uniformities in the magnetization?

Dissipationless Anomalous Hall Current in the Ferromagnetic Spinel $CuCr_2Se_{4-x}Br_x$.

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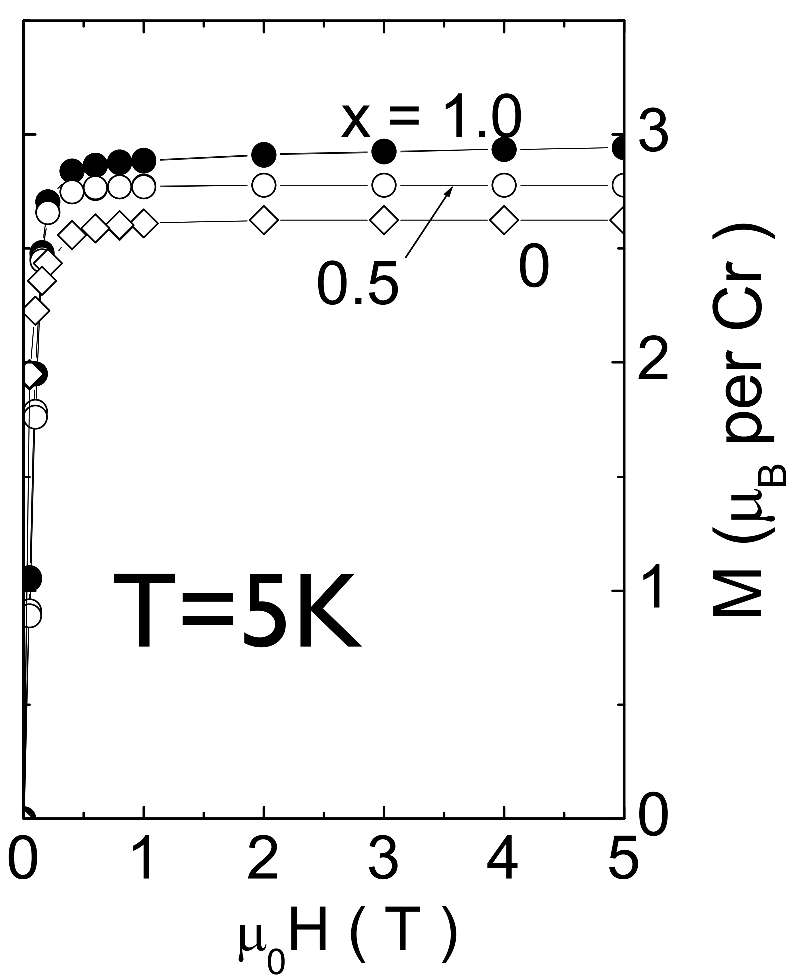
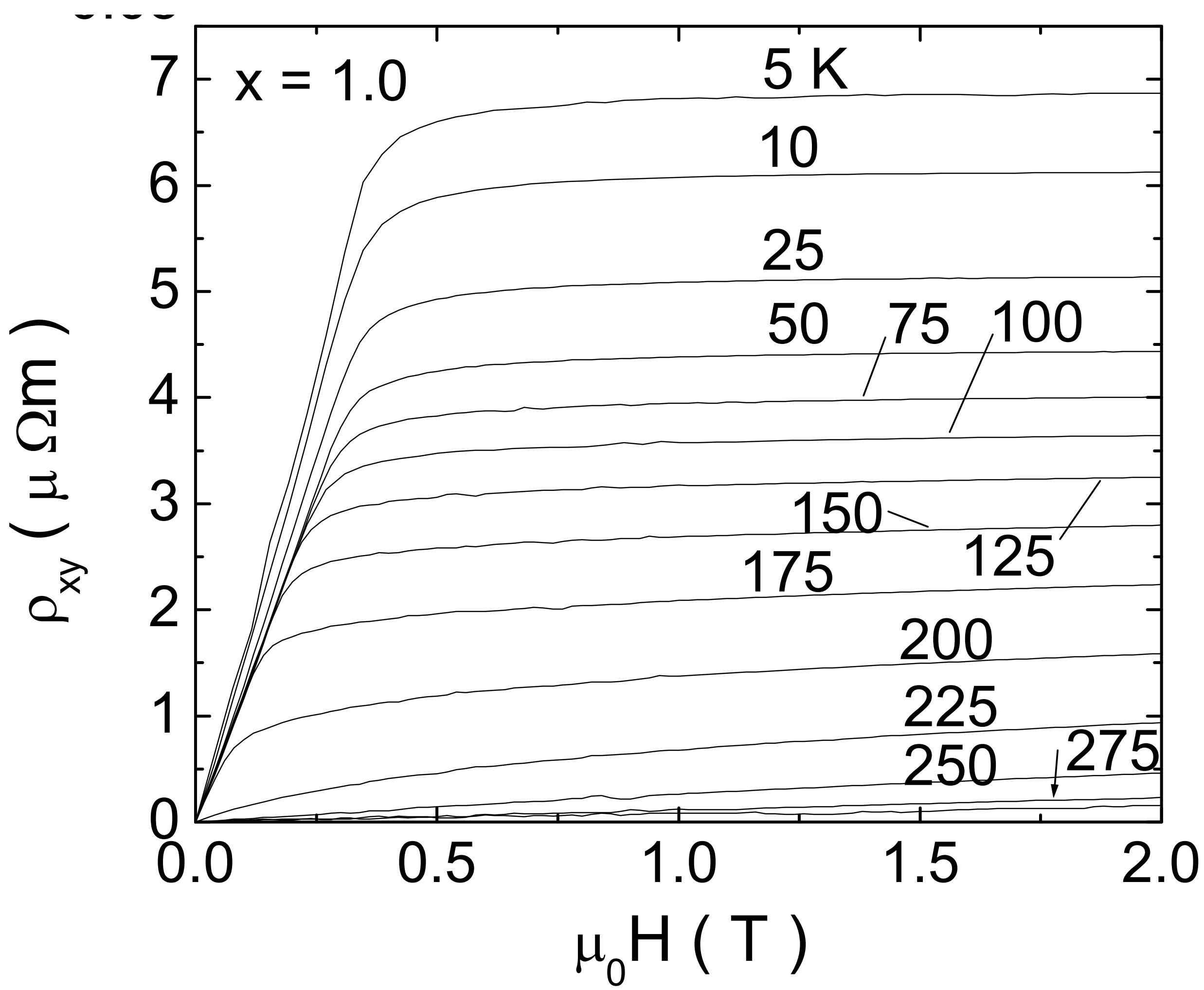




example of a very large AHE

- Karplus and Luttinger (1954): proposed an intrinsic bandstructure explanation, involving Bloch states, spin-orbit coupling and the imbalance between majority and minority spin carriers.

- A key ingredient of KL is an extra "anomalous velocity" of the electrons in addition to the usual group velocity.

- More recently, the KL "anomalous velocity" was reinterpreted in modern language as a "Berry phase" effect.

- In fact, while the KL formula looks like a band-structure effect, I have now found it is a new fundamental Fermi liquid theory feature (possibly combined with a quantum Hall effect.)

various explanations of the anomalous Hall effect

- Intrinsic dissipationless antisymmetric part of the conductivity tensor of the ideal periodic material (Karplus-Luttinger term)

- Magnetic "skew" and "sidejump" scattering from impurities (or inhomogeneous textures of the ferromagetic order parameter), so amplitudes for spin-orbit scattering to "left" and "right" (determined relative to $v_F \times S$) are inequivalent (violate so-called "detailed balance")

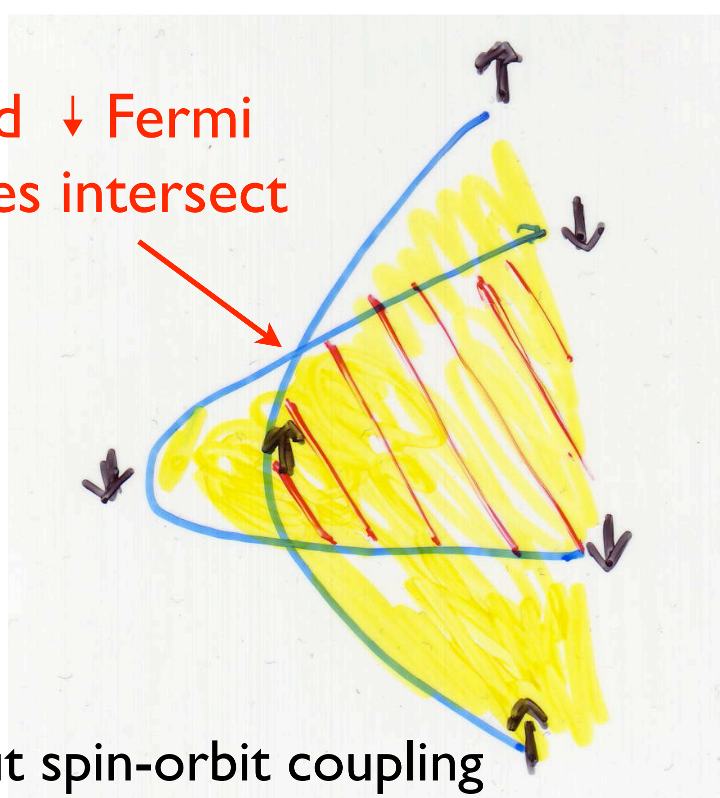
In different regimes of temperature and purity, either of these mechanisms may dominate. In many systems, the controversial Karplus-Luttinger mechanism dominates.

Physical origin of Berry curvature in Ferromagnetic bands

- In a naive Stoner-type theory (neglecting spin-orbit coupling) of ferromagnetic metals, the bands are "exchange-split" into bands of "majority" and "minority" spin carriers.

- In this picture, the majority and minority spin Fermi surfaces are independent, and can intersect:

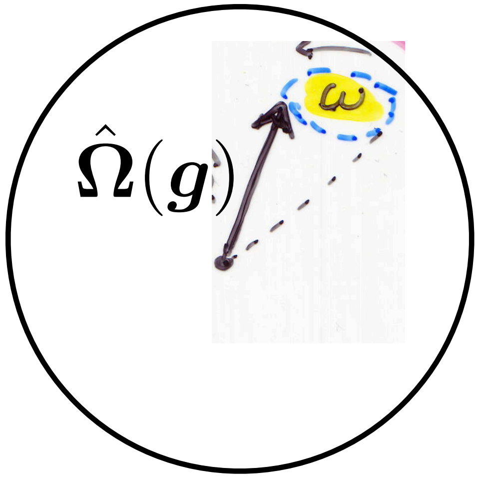
↑ and ↓ Fermi surfaces intersect



without spin-orbit coupling

even though weak, SOC dominates near "avoided intersections" of the Fermi surface, where it causes rapid variation of quasiparticle spin with k_F

Berry curvature due to spin rotations:



- g-dependent spin direction: $\hat{\boldsymbol{\Omega}}(\boldsymbol{g})$

$$\mathcal{F}_{\mu\nu}(\boldsymbol{g}) = \frac{S}{4\pi}\hat{\boldsymbol{\Omega}}(\boldsymbol{g}) \cdot \partial_\mu \hat{\boldsymbol{\Omega}}(\boldsymbol{g}) \times \partial_\nu \hat{\boldsymbol{\Omega}}(\boldsymbol{g})$$

- The Berry phase accumulated as a spin-S rotates is S times the solid angle enclosed by the path of its direction $\boldsymbol{\Omega}$ on the unit sphere.

- (Here "g" is position on the Fermi surface, S= *½)*

Semiclassical dynamics of Bloch electrons

Motion of the center of a wavepacket of band-n electrons centered at $\boldsymbol{k}$ in reciprocal space and $\boldsymbol{r}$ in real space:

(Sundaram and Niu 1999)

$$\boxed{\begin{aligned} \hbar\frac{dk_a}{dt} &= eE_a + eF_{ab}\frac{dr^b}{dt} \\ \hbar\frac{dr^a}{dt} &= \nabla_k^a \varepsilon_n(\boldsymbol{k}) + \hbar\mathcal{F}_n^{ab}(\boldsymbol{k})\frac{dk_b}{dt} \end{aligned}}$$

write magnetic flux density
as an antisymmetric tensor

$$F_{ab}(\boldsymbol{r}) = \epsilon_{abc}B^c(\boldsymbol{r})$$

Karplus and Luttinger 1954

Note the "anomalous velocity" term!
(in addition to the group velocity)

- The Berry curvature acts in k-space like a **magnetic flux density** acts in real space.
- Covariant notation $\boldsymbol{k_a}$, $\boldsymbol{r^a}$ is used here to emphasize the **duality** between k-space and r-space, and expose metric dependence or independence ($a \in \{x,y,z\}$).

- A useful way to write the semiclassical dynamics:

$$\epsilon_{abc}B^c(\boldsymbol{r})$$

$$\hbar \begin{pmatrix} (e/\hbar)F_{ab}(\boldsymbol{r}) & -\delta_a^b \\ \delta_b^a & \mathcal{F}^{ab}(\boldsymbol{k}) \end{pmatrix} \frac{d}{dt} \begin{pmatrix} r^b \\ k_b \end{pmatrix} = \begin{pmatrix} \nabla_a V(\boldsymbol{r}) \\ \nabla_k^a \varepsilon_n(\boldsymbol{k}) \end{pmatrix}$$

$$-i \begin{pmatrix} [k_a, k_b] & [k_a, r^b] \\ [r^a, k_b] & [r^a, r^b] \end{pmatrix}$$

commutators of variables
(symplectic form, Poisson brackets)

$$\begin{pmatrix} \nabla_a H(\boldsymbol{r}, \boldsymbol{k}) \\ \nabla_k^a H(\boldsymbol{r}, \boldsymbol{k}) \end{pmatrix}$$

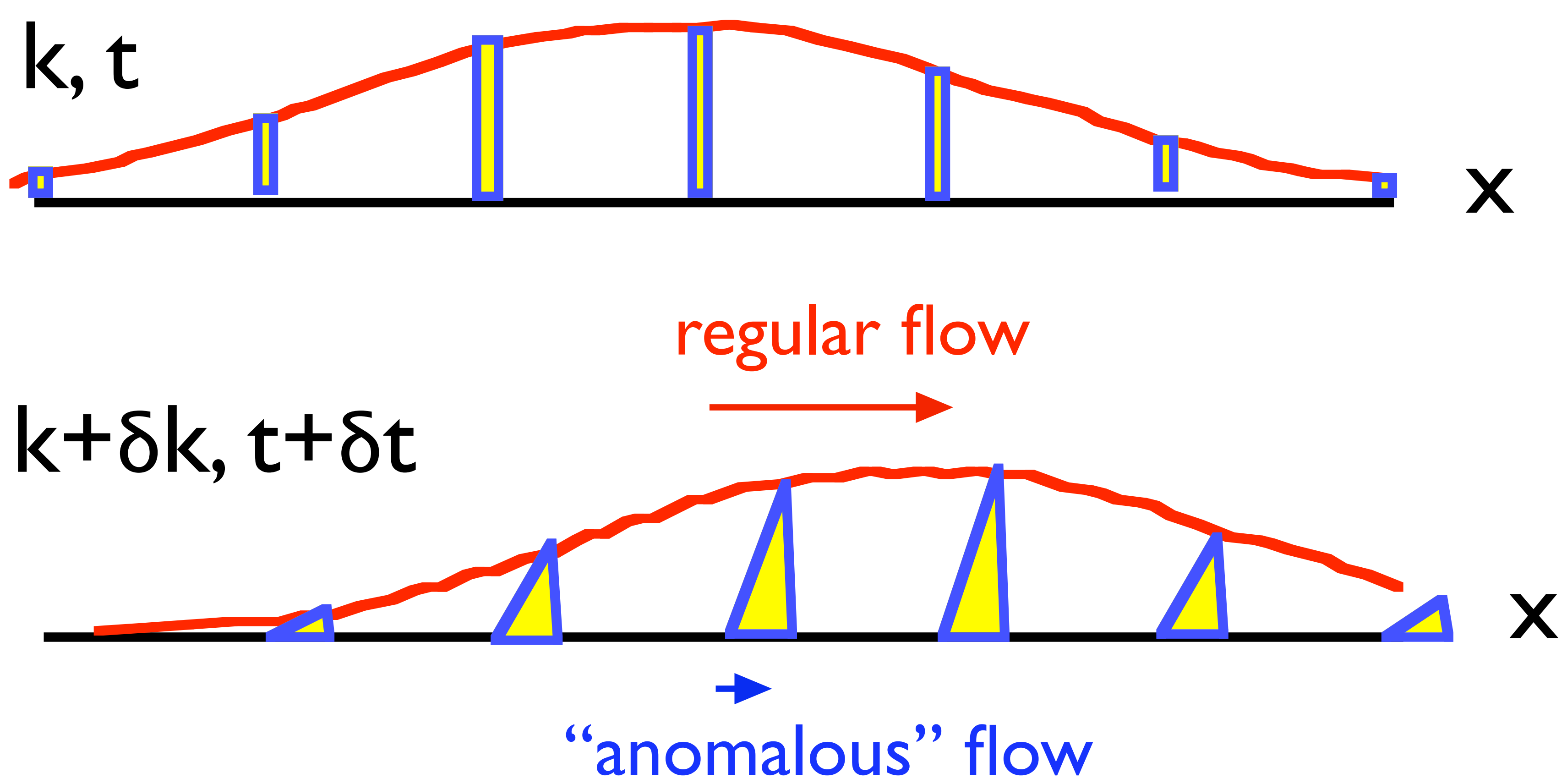
$$H(\boldsymbol{r}, \boldsymbol{k}) = \varepsilon_n(\boldsymbol{k}) + V(\boldsymbol{r})$$

determinant (Jacobian) of the symplectic form :

$$\boxed{\det |\ldots| = 1 + \epsilon_{abc}\mathcal{F}^{ab}(\boldsymbol{k}) \left(\frac{eB^c(\boldsymbol{r})}{\hbar} \right)}$$

modifies phase space volume integral (will use later)

Current flow as a Bloch wavepacket is accelerated



- If the Bloch vector $\boldsymbol{k}$ (and thus the periodic factor in the Bloch state) is changing with time, the current is the ***sum*** of a ***group-velocity term*** (motion of the envelope of the wave packet of Bloch states) and an ***"anomalous" term*** (motion of the $\boldsymbol{k}$-dependent charge distribution inside the unit cell)

- If both ***inversion and time-reversal symmetry are present***, the charge distribution in the unit cell remains inversion symmetric as $\boldsymbol{k}$ changes, and ***the anomalous velocity term vanishes***.

The DC conductivity tensor can be divided into a symmetric Ohmic (dissipative) part and an antisymmetric non-dissipative Hall part:

$$\sigma^{ab} = \sigma^{ab}_{\mathrm{Ohm}} + \sigma^{ab}_{\mathrm{Hall}}$$

In the limit T $\rightarrow$0, there are a number of exact statements that can be made about the DC Hall conductivity of a translationally-invariant system.

For non-interacting Bloch electrons, the Kubo formula gives an intrinsic Hall conductivity (in both 2D and 3D)

$$\sigma^{ab}_{\mathrm{Hall}} = \frac{e^2}{\hbar}\frac{1}{V_D}\sum_{n\boldsymbol{k}} \mathcal{F}^{ab}_n(\boldsymbol{k})\Theta(\varepsilon_F - \varepsilon_n(\boldsymbol{k}))$$

This is given in terms of the total Berry curvature of occupied states with band index n and Bloch vector k.

If the Fermi energy is in a gap, so every band is either empty or full, this is a topological invariant:
(integer quantized Hall effect)

$$\sigma^{xy} = \frac{e^2}{\hbar}\frac{1}{2\pi}\nu \quad \nu = \text{an integer}(2D)$$

TKNN formula

$$\sigma^{ab} = \frac{e^2}{\hbar}\frac{1}{(2\pi)^2}\epsilon^{abc}K_c \quad \boldsymbol{K} = \text{a reciprocal vector } \boldsymbol{G}\ (3D)$$

In 3D $\boldsymbol{G} = \nu\boldsymbol{G}_0$, where $\boldsymbol{G}_0$ indexes a family of lattice planes with a 2D QHE.

Implication: If in 2D, ν is NOT an integer, the non-integer part MUST BE A FERMI SURFACE PROPERTY!

In 3D, any part of K modulo a reciprocal vector also must be a Fermi surface property!

3D zero-field Quantized Hall Effect

- Families of lattice planes in a 3D periodic structure are indexed by a primitive reciprocal lattice vector $\boldsymbol{G}^0$. ***Each plane*** is a 2D periodic system that could exhibit a 2D QHE with integer "filling factor" ν. This adds up to a 3D Hall conductivity with "***Hall vector***" $\boldsymbol{K} = \nu\boldsymbol{G}^0 = \boldsymbol{G}_H$, a reciprocal vector (in general, non-primitive).

- Such a system will have a gap at the Fermi level, with a number of completely-filled Bloch state bands. The "Hall vector" in this case is a sum of topological invariants of the non-degenerate filled bands (or groups of bands linked by degeneracies).

$$\boldsymbol{G}_H = \sum_n{}' \boldsymbol{G}_n .$$ (sum over filled bands)

$$\epsilon^{abc} G_{nc} = \frac{1}{2\pi} \int_{\mathrm{BZ}} d^3\boldsymbol{k}\, \mathcal{F}_n^{ab}(\boldsymbol{k})$$ (band n "Chern vector")

a 3x3 antisymmetric matrix can always be brought to "symplectic diagonal form" $\begin{pmatrix} 0 & \mathcal{F} & 0 \\ -\mathcal{F} & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$

2D case: "Bohm-Aharonov in k-space"

$$\sigma^{xy} = \frac{e^2}{\hbar}\frac{1}{(2\pi)^2}\int d^2k\ (\nabla_k \times \mathcal{A}(\boldsymbol{k}))\, n(\boldsymbol{k})$$

$$\sigma^{xy} = \frac{e^2}{\hbar}\frac{1}{(2\pi)^2}\oint_{\mathrm{FS}} \mathcal{A}(\boldsymbol{k})\cdot d\boldsymbol{k}$$

$$\boxed{\sigma^{xy} = \frac{e^2}{h}\left(\frac{\Phi_F^{\mathrm{Berry}}}{2\pi}\right)}$$

- The Berry phase for moving a quasiparticle around the Fermi surface is only defined modulo 2π:
- Only the <u>non-quantized</u> part of the Hall conductivity is defined by the Fermi surface!

- even the quantized part of Hall conductance is determined at the Fermi energy (in edge states necessarily present when there are fully-occupied bands with non-trivial topology)

- All transport occurs AT the Fermi level, not in "states deep below the Fermi energy". (transport is NOT diamagnetism!)

[2D zero-field Quantized Hall Effect]

FDMH, Phys. Rev. Lett. 61, 2015 (1988).

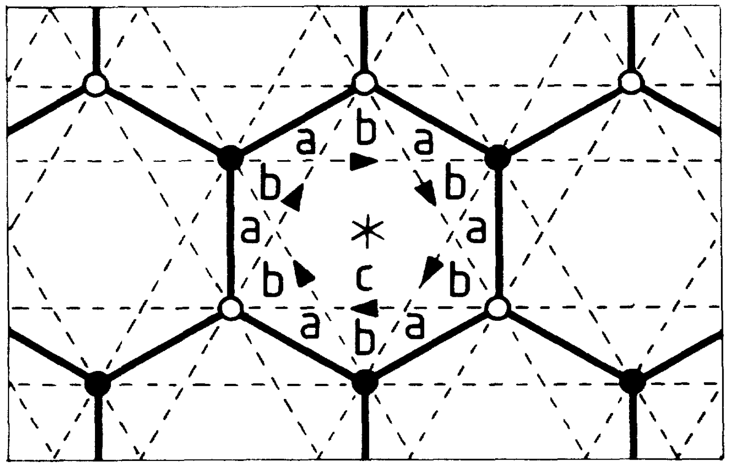


FIG. 1. The honeycomb-net model ("2D graphite") showing nearest-neighbor bonds (solid lines) and second-neighbor bonds (dashed lines). Open and solid points, respectively, mark the *A* and *B* sublattice sites. The Wigner-Seitz unit cell is conveniently centered on the point of sixfold rotation symmetry (marked "*") and is then bounded by the hexagon of nearest-neighbor bonds. Arrows on second-neighbor bonds mark the directions of positive phase hopping in the state with broken time-reversal invariance.

- 2D quantized Hall effect: $\sigma^{xy} = \nu e^2/h$. In the absence of interactions between the particles, ν must be an <u>integer</u>. There are no current-carrying states at the Fermi level in the interior of a QHE system (all such states are localized on its <u>edge).</u>

- The 2D integer QHE does NOT require Landau levels, and can occur if time-reversal symmetry is broken even if there is no net magnetic flux through the unit cell of a periodic system. (This was first demonstrated in an explicit "graphene" model shown at the right.).

- Electronic states are "simple" Bloch states! (real first-neighbor hopping t_1, complex second-neighbor hopping $t_2 e^{i\varphi}$, alternating onsite potential M.)

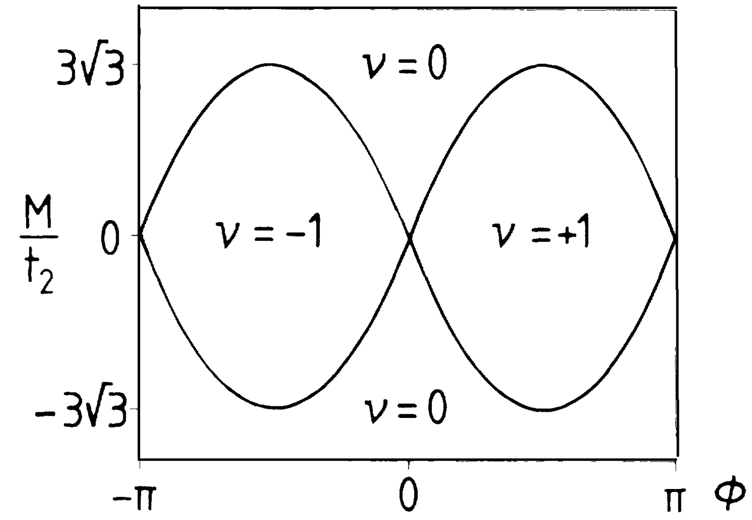
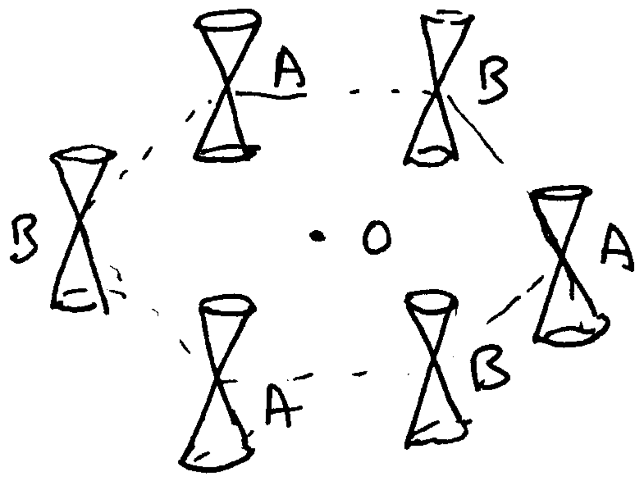
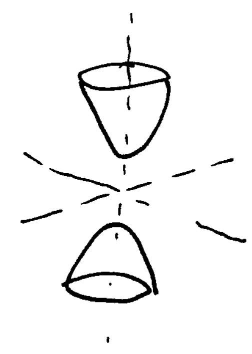


FIG. 2. Phase diagram of the spinless electron model with $|t_2/t_1| < \frac{1}{3}$. Zero-field quantum Hall effect phases ($\nu = \pm 1$, where $\sigma^{xy} = \nu e^2/h$) occur if $|M/t_2| < 3\sqrt{3}|\sin\phi|$. This figure assumes that t_2 is positive; if it is negative, ν changes sign. At the phase boundaries separating the anomalous and normal ($\nu = 0$) semiconductor phases, the low-energy excitations of the model simulate undoubled massless chiral relativistic fermions.

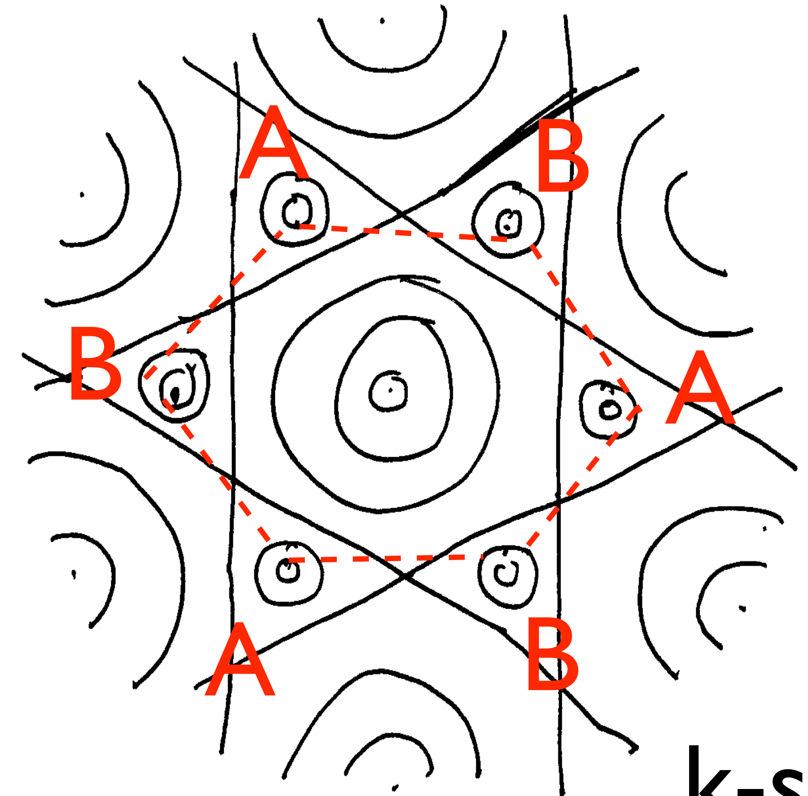
2D “graphene” bandstructure



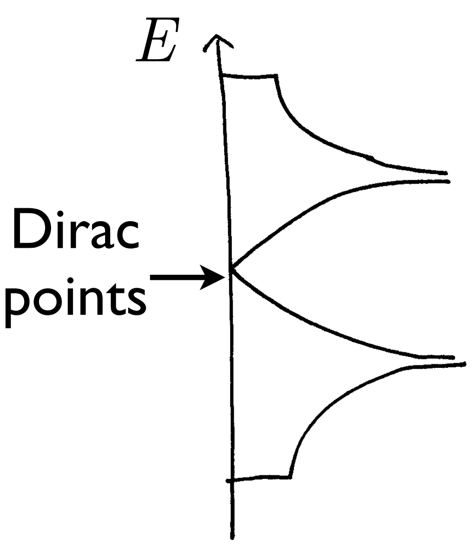
two distinct “Dirac points” (at corners of hexagonal Brillouin zone)



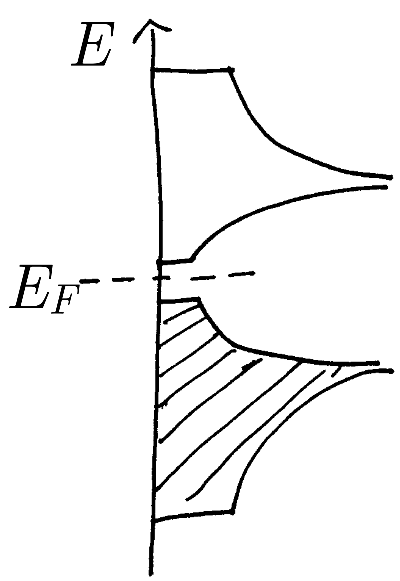
Breaking either inversion (I) or time-reversal (T) symmetry opens a “mass gap” at Dirac points.)



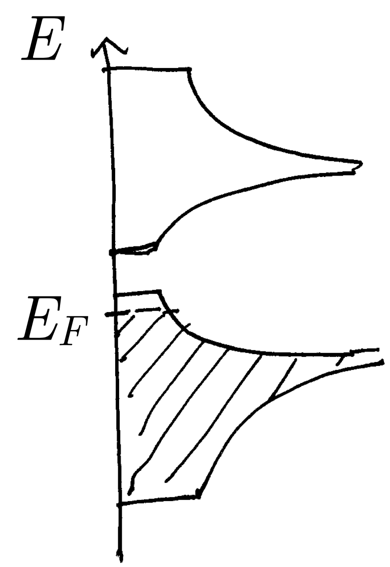
k-space



density of states (massless)



massive case (bulk insulator)



massive case (bulk metal)

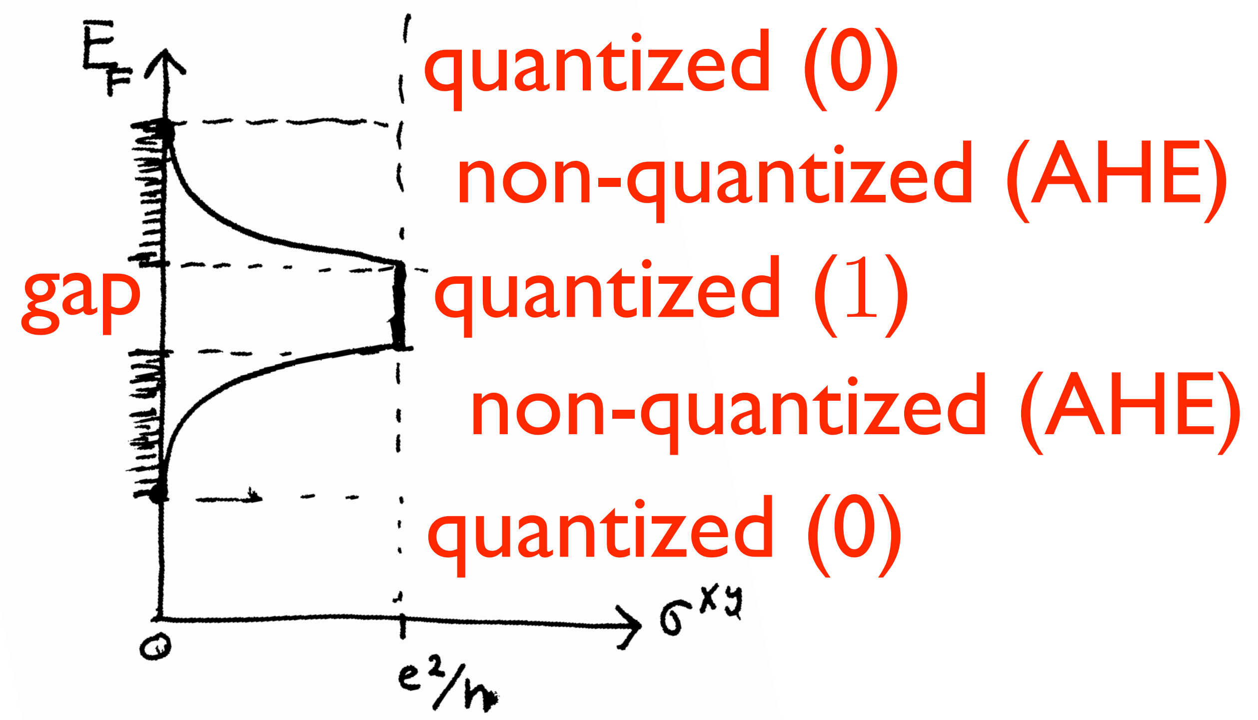
Break only T: $m_A = m_B$

same sign Berry curvature near A and B points

Break only I: $m_A = -m_B$

opposite sign Berry curvature near A and B points

- Intrinsic (Karplus Luttinger) Hall conductivity interpolates between quantized Hall conductance from edge states

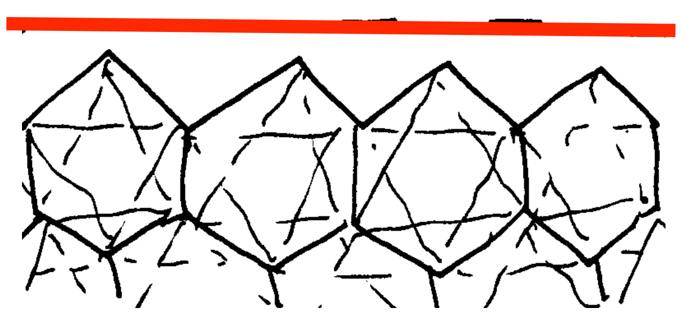


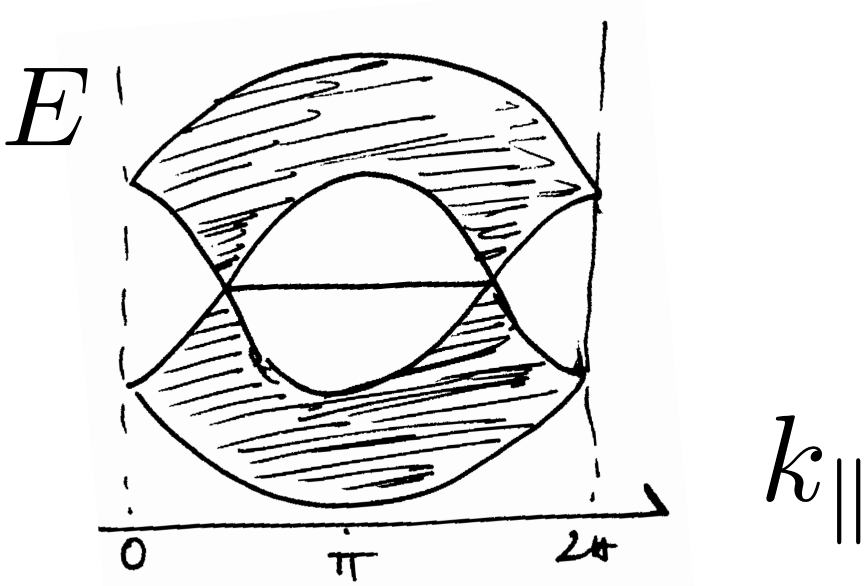
Graphene model with second neighbor hopping is very useful!

- Quantum Hall effect with simple Bloch states
- Used for anomalous Hall effect studies(Nagaosa), add disorder etc.
- used for testing/developing fundamental band-stucture formulas for orbital magnetization (Vanderbilt)
- Quantum Spin Hall effect (Kane and Mele)
- Analog system for photonic edge states (Haldane and Raghu)

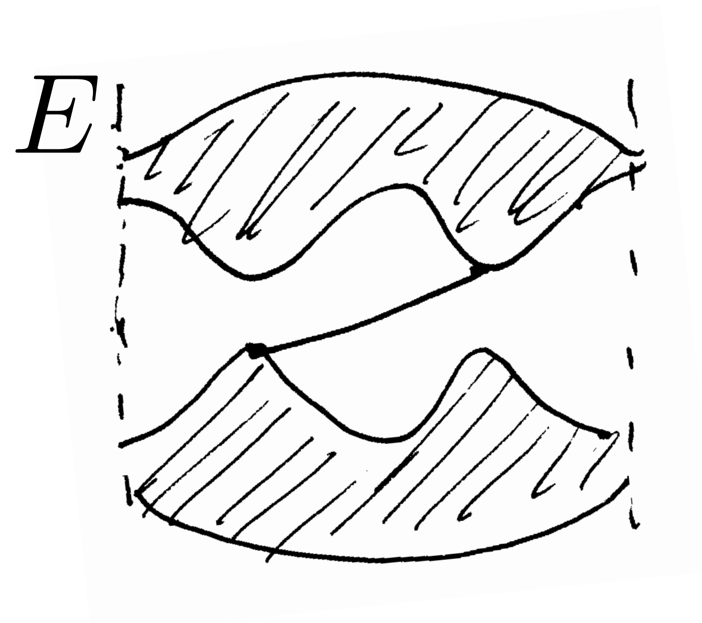
- graphene edge states (zigzag edge)

edge

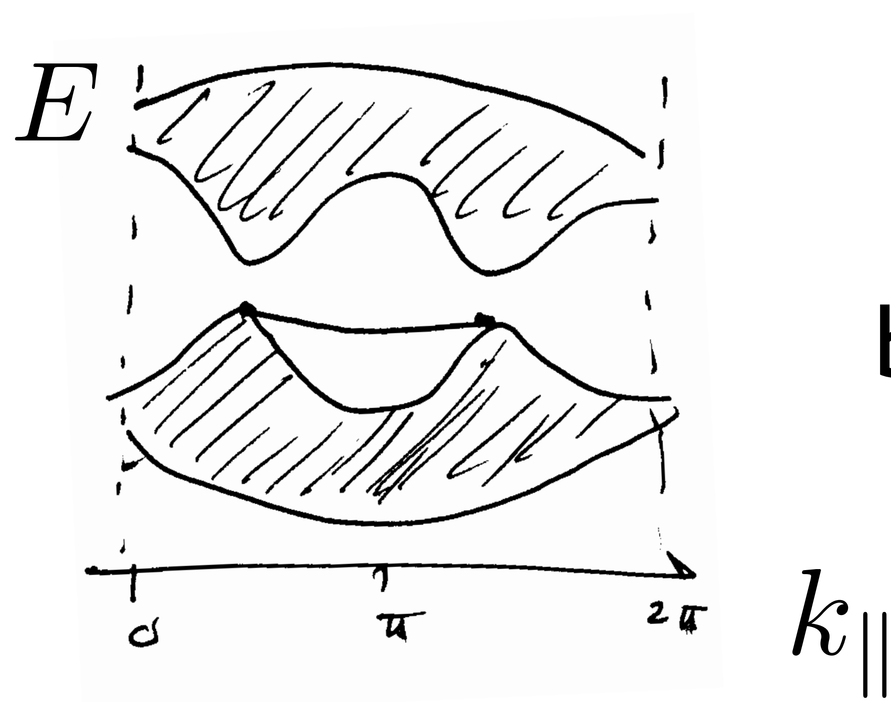




gapless case



broken T



broken I

non-quantized part of 3D case can also be expressed as a Fermi surface integral

- **There is a separate contribution to the Hall conductivity from each distinct Fermi surface manifold.**

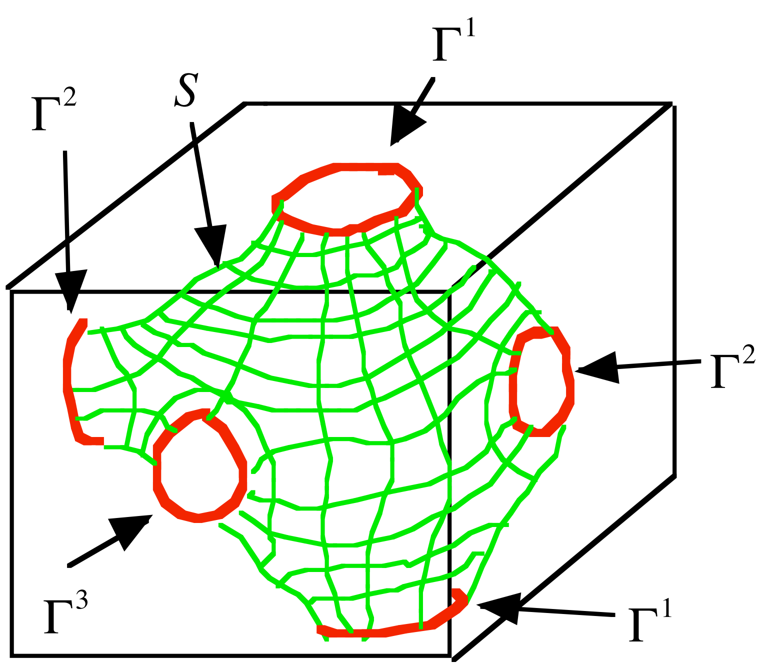
- Intersections with the Brillouin-zone boundary need to be taken into account.

"Anomalous Hall vector":

$$\boldsymbol{K} = \sum_\alpha \boldsymbol{K}_\alpha (\text{modulo } \boldsymbol{G}) \qquad \boldsymbol{K}_\alpha = \frac{1}{2\pi}\left(\int d^2\mathcal{F}\, \boldsymbol{k}_F + \sum_{i=1}^{d_\alpha^G} \boldsymbol{G}_i \oint_{\Gamma_\alpha^i} d\mathcal{A} \right)$$

integral of Fermi vector weighted by Berry curvature on FS

Berry phase around FS intersection with BZ boundary



This is ambiguous up to a reciprocal vector, which is a non-FLT quantized Hall edge-state contribution

First Principles Calculation of Anomalous Hall Conductivity in Ferromagnetic bcc Fe

Yugui Yao[1,2,3], L. Kleinman[1], A. H. MacDonald[1], Jairo Sinova[4,1],
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tions to Ω^z. Only when the Fermi surface lies in a spin-orbit induced gap is there a large contribution. This can be seen in Fig. 3 where the Berry curvature along lines in $\mathbf{k}$-space is compared with energy bands near E_F and in Fig. 4 where it is compared with the intersection of the Fermi surface with the central (010) plane in the Brillouin zone.

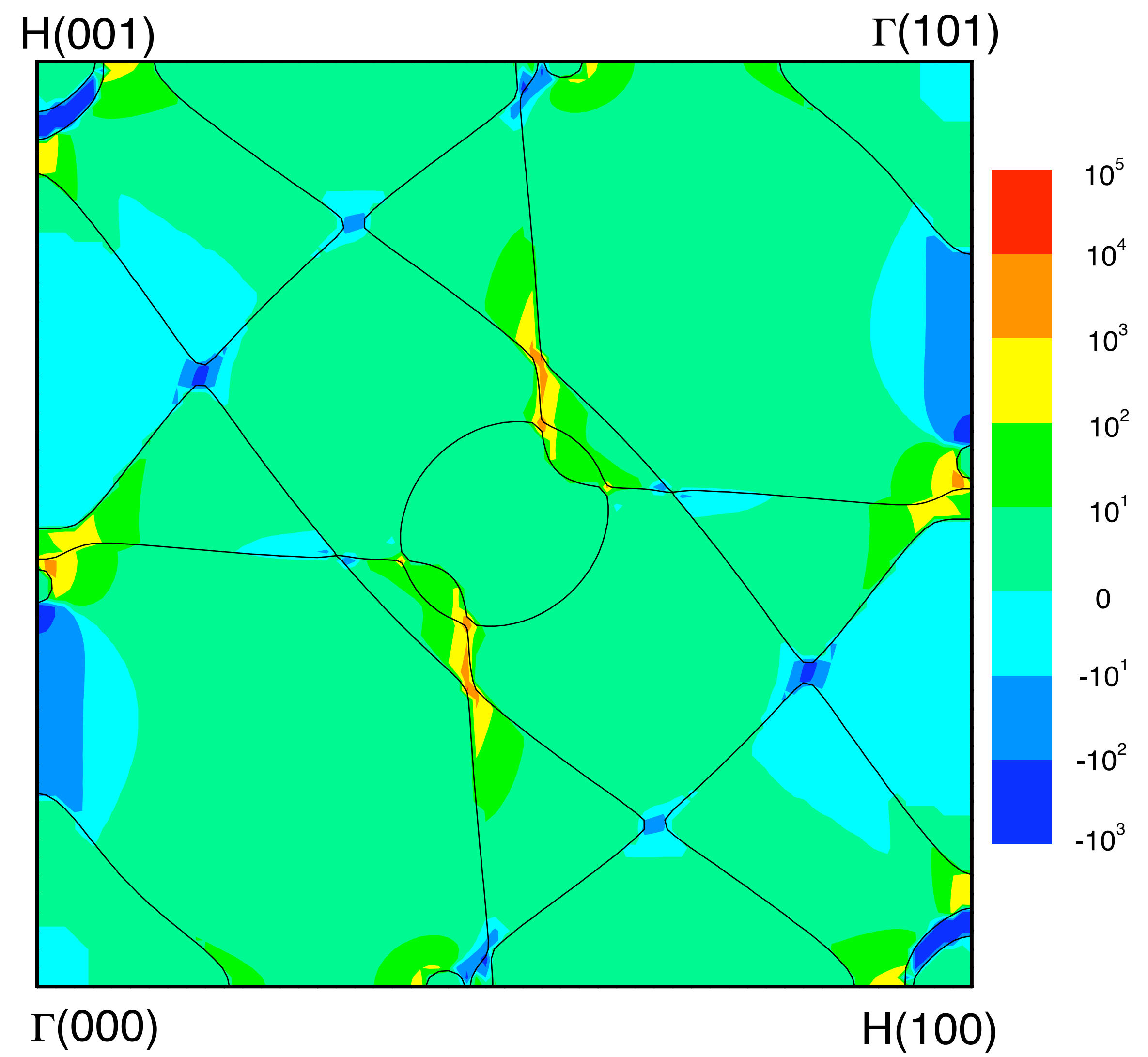


FIG. 4: (010) plane Fermi-surface (solid lines) and Berry curvature $-\Omega^z(\mathbf{k})$ (color map). $-\Omega_z$ is in atomic units.

This calculation sampled ALL states below the Fermi level (unnecessary work!) but shows how avoided Fermi surface intersections provide the dominant contributions to the KL formula.

Bands with both time-reversal and spatial-inversion symmetry:

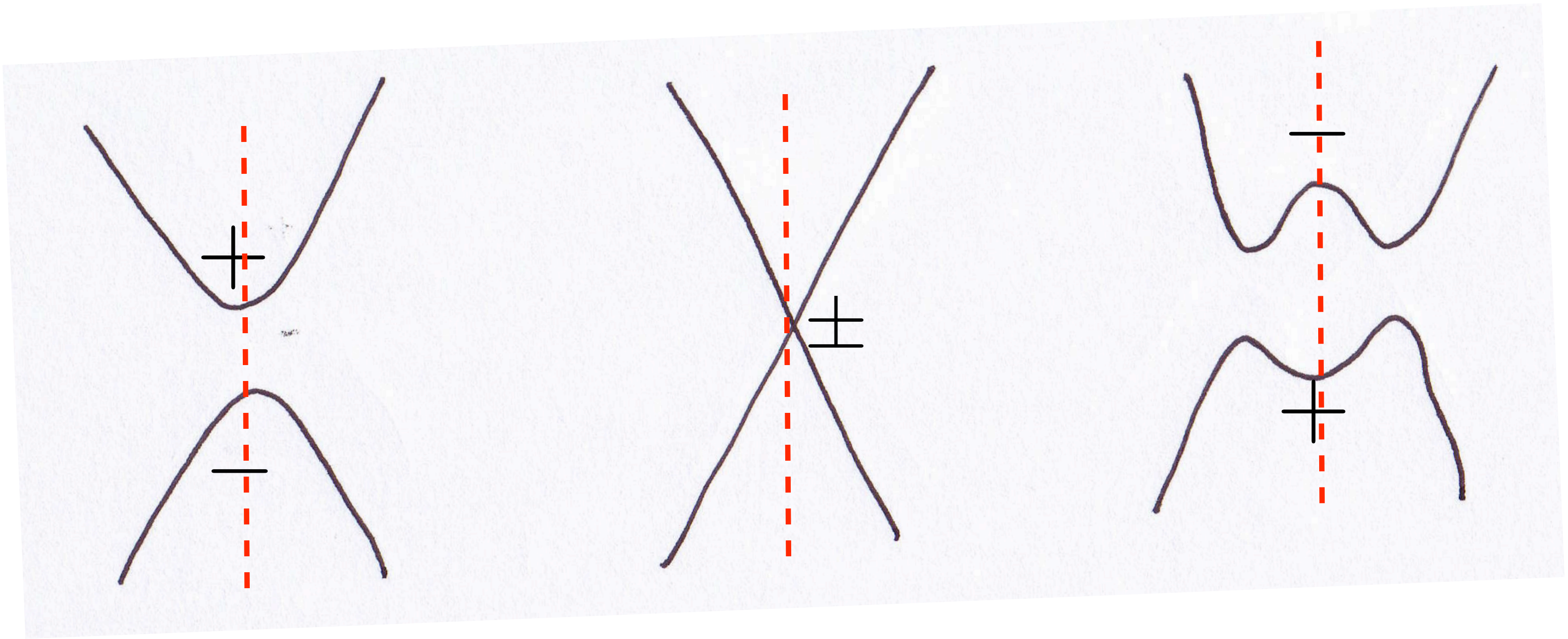
- Bands are doubly-degenerate at generic points in the Brillouin zone
- Bands at special k-points where $2\boldsymbol{k}_j = \boldsymbol{G}$ are classified by **inversion symmetry** $I_i(\boldsymbol{k}_j) = +1$ or -1 about inversion center i in the real-space unit cell.
- In 2D (3D) there are 4 (8) special k-points and 4 (8) distinct inversion centers; the product over all bands below the Fermi energy is

$$\eta_0 = \prod_j I_i(\boldsymbol{k}_j) = \pm 1$$

Fu and Kane, 2006

- In 2D and above this is independent of which inversion center i is chosen

This is clearly a "topological invariant", but Kane and Fu's recent (2006) result shows the not-so-obvious fact that it must have the value $+1$ in the absence of spin-orbit coupling.



η_0 is a topological invariant because it cannot change without the gap closing

At special k-points, it is possible to "fine-tune" bands with opposite inversion quantum numbers to have an "accidental degeneracy" by varying a **single** parameter.

Topological invariants of Bloch bands:

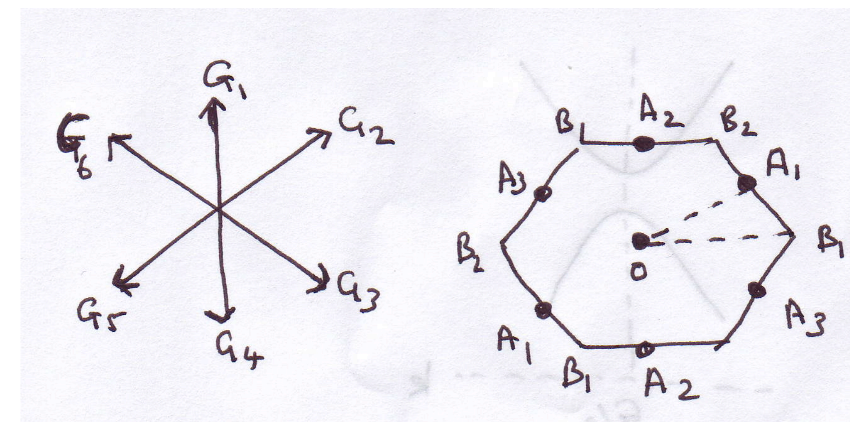
- cannot change unless the energy gap between bands closes and reopens:
- The integer "Chern number" (First Chern Class) classifies Bloch bands with **broken time-reversal symmetry:**
- If there is a gap at the Fermi energy, a non-zero total **Chern number** of 2D bands below the Fermi energy implies that:

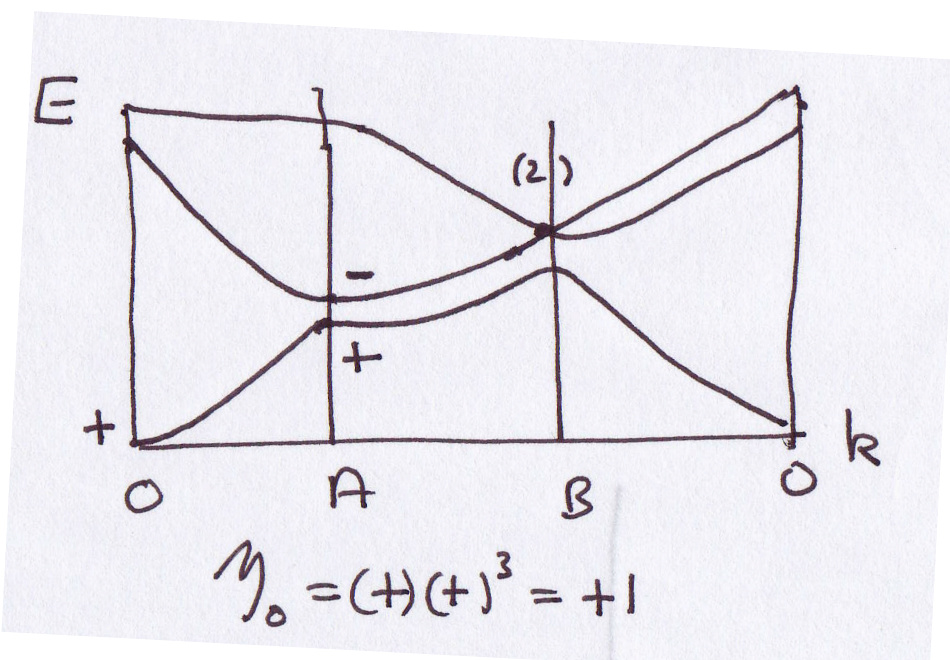
There is an (integer) quantum Hall effect

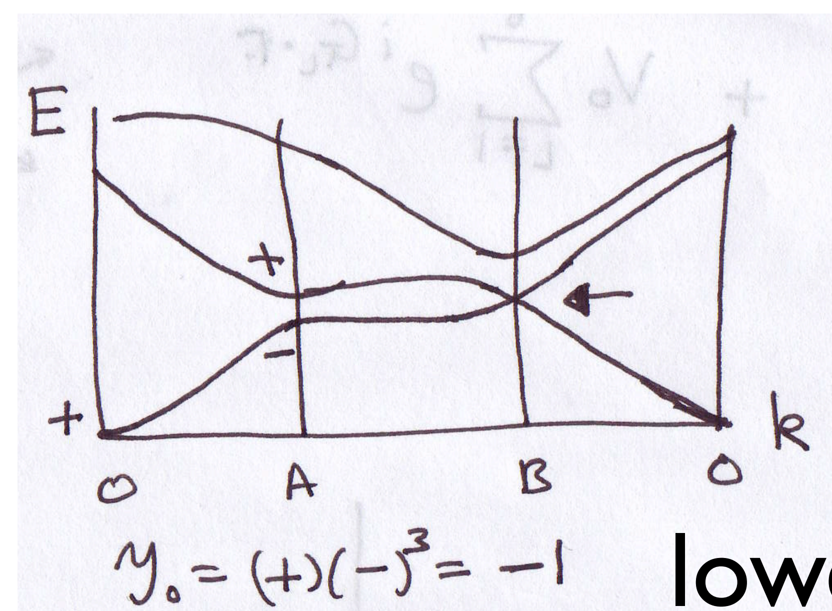
There are gapless chiral edge states at the edge of the system.

- example (with no spin-orbit coupling)

$$H = \frac{p^2}{2m} + V_0 \sum_{i=1}^{6} e^{i\boldsymbol{G}_i \cdot \boldsymbol{r}}$$







$V_0 < 0$

lowest band has η_0 = $+1$

$V_0 > 0$

lowest band has η_0 = -1

but no gap!

Berry curvature and the Z2 invariant when inversion symmetry is broken.

- Kane and Mele gave a formulation in terms of the zeroes of a "Pfaffian matrix"
- Kane and Fu gave a formulation in terms of what they identify as a Berry curvature of a determinant of occupied bands
- I will now give a formulation in terms of the Berry curvature structure of individual Bloch states, using the Berry curvature as defined by their semiclassical dynamics.

- Key point: these expressions are not **definitions** of the topological invariant, which fundamentally measures whether an even or an odd number of Dirac points have crossed the Fermi level as the band structure has evolved from one with no spin-orbit coupling.
- Instead, they are **sum rules** involving the Berry curvature (or Pfaffian zeroes)
- Indeed, the invariant is a property of the Hamiltonian alone, while the Berry curvature depends on **extra information about its embedding in Euclidean space**.

$c^{\dagger}_{\boldsymbol{R}\alpha}$ ← Local basis: orbital α in unit cell $\boldsymbol{R}$

$$H^0 = \sum_{\boldsymbol{R},\alpha;\boldsymbol{R}'\alpha'} h_{\alpha\alpha'}(\boldsymbol{R}-\boldsymbol{R}')c^{\dagger}_{\boldsymbol{R}\alpha}c_{\boldsymbol{R}'\alpha'}$$

$$|\Psi_n(\boldsymbol{k})\rangle = \sum_{\boldsymbol{R}\alpha} u_{n\alpha}(\boldsymbol{k})e^{i\boldsymbol{k}\cdot(\boldsymbol{R}+\boldsymbol{r}_\alpha)}|\boldsymbol{R}\alpha\rangle$$

Hamiltonian and Bloch states depend on the matrix-elements $h_{\alpha\alpha'}(\boldsymbol{R})$

Bloch states and Berry curvature <u>also</u> depend on the positions r_α in the unit cell.

- varying the nominal orbital positions in the unit cell *without* changing the matrix elements changes the Berry curvature, <u>**but does not affect the topological invariants.**</u>

- The Berry curvature **of Bloch states** physically represents part of their linear response to <u>**uniform**</u> electromagnetic fields (which cannot be included in a periodic time-independent Hamiltonian)

$$A_n^a(\boldsymbol{k}) = -i\langle\Psi_n(\boldsymbol{k})|\frac{\partial}{\partial k_a}\Psi_n(\boldsymbol{k})\rangle$$

"Berry connection": k-space analog of the magnetic vector potential.

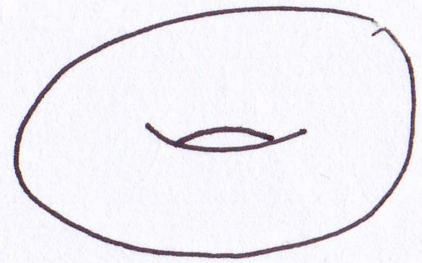
$$F_n^{ab}(\boldsymbol{k}) = \frac{\partial}{\partial k_a}A_n^b(\boldsymbol{k}) - \frac{\partial}{\partial k_b}A_n^a.$$

"Berry curvature": k-space analog of magnetic flux density (gauge invariant)

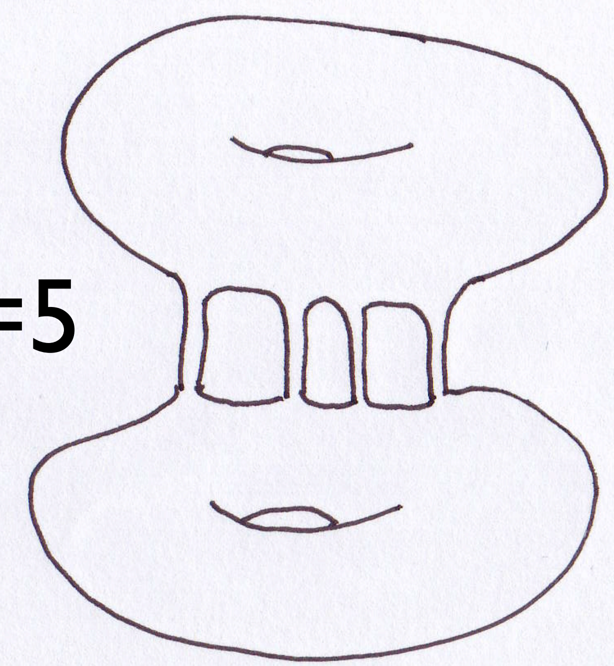
The "anomalous velocity" term in the semiclassical dynamics is

$$\frac{dx^a}{dt} = \frac{1}{\hbar}\nabla_k^a\epsilon_n(\boldsymbol{k}) + F_n^{ab}(\boldsymbol{k})\frac{d\boldsymbol{k}_b}{dt}$$

Topology of 2D bands with time-reversal symmetry



A 2D band with no SOC is topologically a 2-Torus (genus-1 2-manifold)



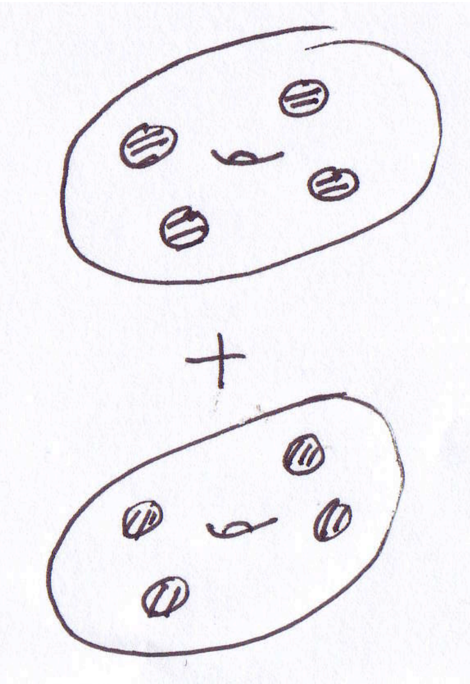
A 2D band with SOC (and no inversion symmetry) is topologically two 2-tori, punctured and joined at the four T-reversal-invariant k-points to make a genus-5 two manifold, (on which every point has a Kramers-conjugate antipode)

basic idea

- If the genus-5 2-manifold is sliced into the upper band and and the lower band, it falls apart into two 2-Tori, each with four "punctures".

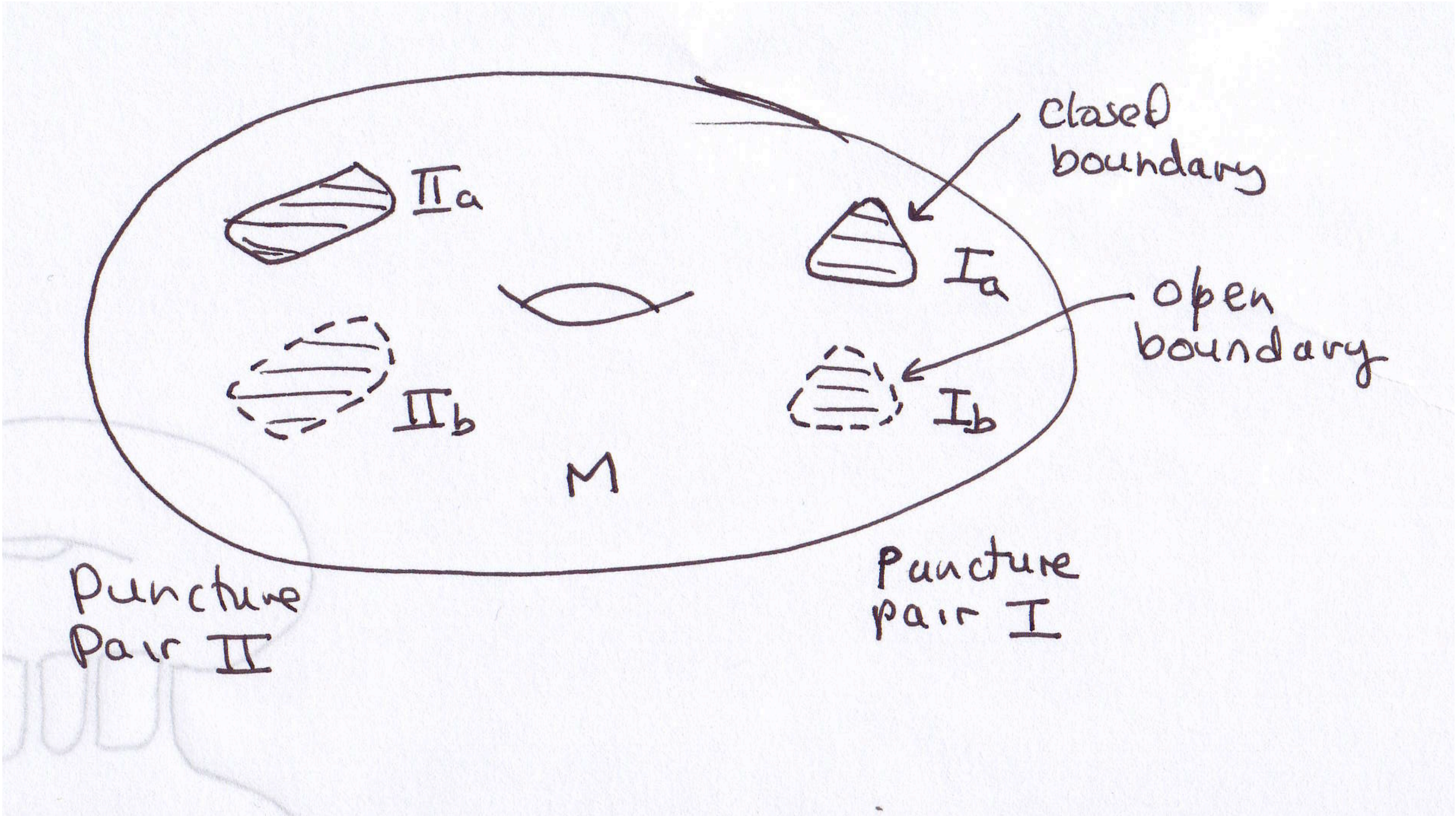
- The edges of the punctures are the 1-manifolds defined by the limit of the Bloch states at the T-invariant k-points, **as a function of the direction they are approached from** in the upper or lower band.

- There is no relation in general between these four punctures (except possible point-group symmetry on square and hexagonal Bravais lattices).



- Instead, divide the genus-5 manifold into two Kramers-conjugate 2-tori with four punctures.   In this case the punctures come in Kramers-conjugate pairs...

Matched pairs of punctures on a Kramers-divided double-band.



- no pairs of points on this manifold are Kramers conjugates
- For each pair of "puncture boundaries", one is open, one is closed.
- The puncture boundaries are topologically non-trivial paths on the uncut genus-5 manifold.

- On an unpunctured 2-manifold $\mathcal{M}$

$$\int_{\mathcal{M}} d^2 F = 2\pi \times \text{integer} \qquad e^{i\int_{\mathcal{M}} d^2 F} = 1$$

- On a punctured 2-manifold with puncture boundaries $\partial\mathcal{M}_i$

$$e^{i\int_{\mathcal{M}} d^2 F} = \prod_i e^{i\phi_B(\partial M_i)}$$

integral of Berry curvature over manifold

product of Berry phases around the puncture edges

This is just Stokes theorem, exponentiated

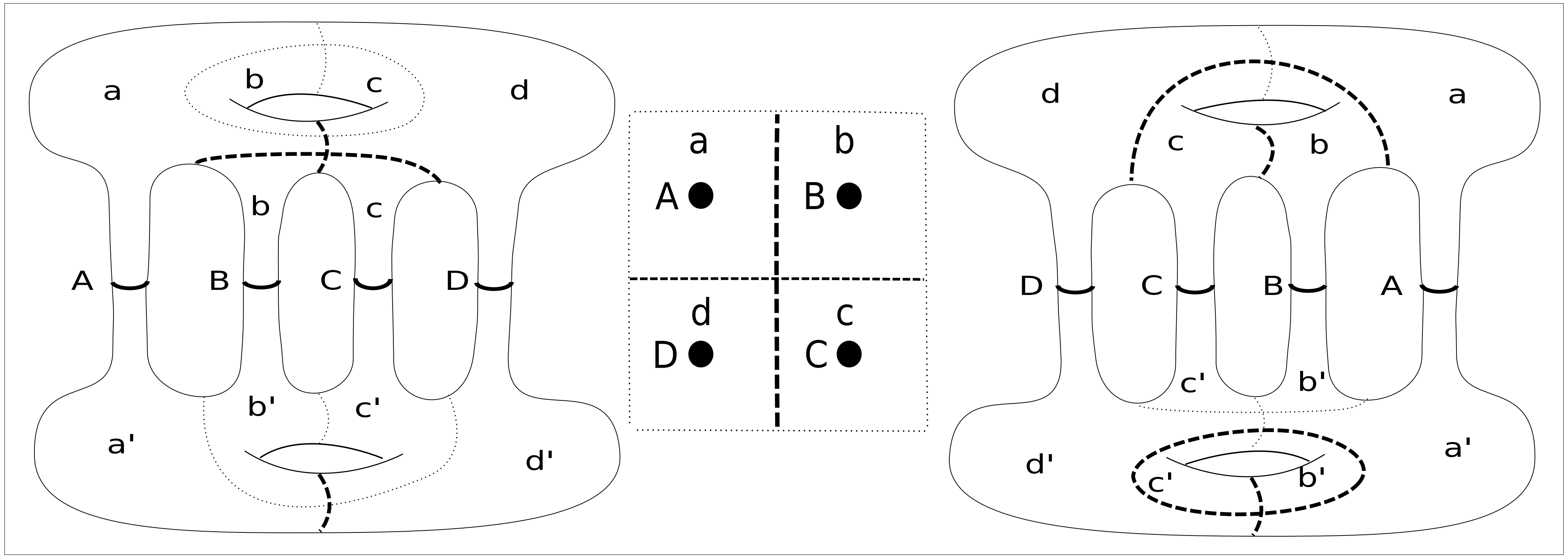
- In general, no topological Chern invariant survives on a punctured manifold.
- Here, each member of a pair of Kramers-conjugate puncture boundaries has the **same** Berry phase factor!

$$e^{i \int_{\mathcal{M}} d^2 F} = \left(\prod_i e^{i\phi_B(\partial M_i)} \right)^2$$

Now take the square root:

$$\boxed{e^{i \frac{1}{2} \int_{\mathcal{M}} d^2 F} = \eta_0 \prod_i e^{i\phi_B(\partial M_i)}}$$

The Z_2 invariant, ± 1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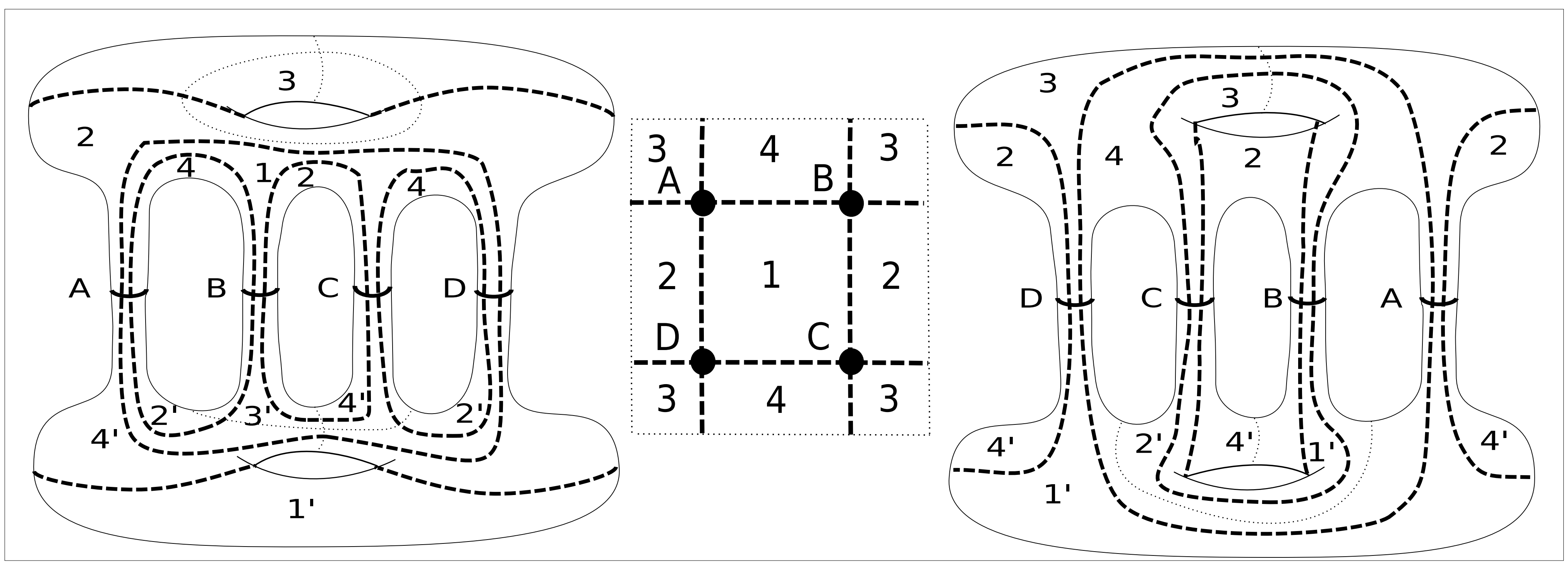
3
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