Quantum geometry in Conducting systems

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- Formal discussion of quantum distance and Berry curvature
- Application to the Anomalous Hall effect in 3D Ferromagnets, and 2D composite Fermions.
- Fermi surface geometry.

geometry of a manifold of quantum states

$$|\Psi(\boldsymbol{g})\rangle = \sum_i \Psi_i(\boldsymbol{g})|i\rangle$$

continuous family of states parameterized by d real parameters

orthonormal fixed basis ($\boldsymbol{g}$-independent)

$\{g^\mu, \mu \in 1, 2, \ldots d\}$

- Berry gauge ambiguity: nothing physical changes if we make a g-dependent gauge change

$$|\Psi(\boldsymbol{g})\rangle \rightarrow e^{i\chi(\boldsymbol{g})}|\Psi(\boldsymbol{g})\rangle$$

Examples of manifolds of states:

- bands of Bloch states (manifold = Brillouin zone)
- Fermi liquid quasiparticles (manifold = Fermi surface in 2D or 3D)
- eigenstates of a family of non-degenerate Hamiltonians (manifold = parameter space of Hamiltonians)
- Coherent states (spin coherent states, Landau level "guiding center" coherent states, etc.)

Hilbert-space distance

$$\boxed{d_p(1,2)^2 = 1 - |\langle\Psi(1)|\Psi(2)\rangle|^p, \quad p \geq 1}$$

- Berry gauge invariant (absolute value)
- obeys the triangle inequality, positivity, etc.
- dimensionless: $\mathrm{d_p(1{,}2)} = 1$ for orthogonal states
- case $\mathrm{p{=}1}$ is Bures-Uhlmann distance, $\mathrm{p{=}2}$ is Hilbert-Schmidt distance, $\mathrm{p{=}\infty}$ is classical ("trivial distance" $\mathrm{d_{ij}} = 1 \text{ for } \mathrm{i{\neq}j}$)
- Eigenstates of Hamiltonian are stationary (only phase changes with time): with this definition of distance, the speed of motion in Hilbert space of a non-eigenstate is

$d(12) = d(21) \geq 0$

$d(12) = 0 \text{ iff } 1 = 2$

$d(12) + d(23) \geq d(13)$

fundamental property of a distance

$$v_p = \frac{(p/2)^{1/2}}{\hbar}(\Delta H)_{rms}$$

$$(\Delta H)^2 \equiv \langle H^2\rangle - \langle H\rangle^2$$

energy variance

- a generic quantum state on a manifold induces both a Riemannian metric (through its distance property) and a $U(1)$ gauge field (the "Berry connection")("unitary" case)

(Hermitian) (symmetric) (antisymmetric)

$$\langle D_\mu \Psi(\boldsymbol{g})|D_\nu \Psi(\boldsymbol{g})\rangle = \mathcal{G}_{\mu\nu}(\boldsymbol{g}) + i\mathcal{F}_{\mu\nu}(\boldsymbol{g})$$

covariant derivative

Riemann metric

Berry curvature

- If the states are eigenstates of a family of time-reversal-invariant Hamiltonians, the Berry gauge field is Z(2) ("orthogonal" case, without spin-orbit coupling, or SU(2) ("symplectic" case):

$$\langle D_\mu \Psi_\sigma(\boldsymbol{g})|D_\nu \Psi_{\sigma'}(\boldsymbol{g})\rangle = \mathcal{G}_{\mu\nu}(\boldsymbol{g})\delta_{\sigma\sigma'} + i\mathcal{F}^a_{\mu\nu}(\boldsymbol{g})\sigma^a_{\sigma\sigma'}$$

non-Abelian Berry curvature

Pauli matrix

$$|\Psi(\boldsymbol{g})\rangle = \sum_i \Psi_i(\boldsymbol{g})|i\rangle$$

$$|\partial_\mu\Psi(\boldsymbol{g})\rangle \equiv \sum_i \frac{\partial}{\partial g^\mu}\Psi_i(\boldsymbol{g})|i\rangle$$

- regular derivative

$$\mathcal{A}_\mu(\boldsymbol{g}) = -i\langle\Psi(\boldsymbol{g})|\partial_\mu\Psi(\boldsymbol{g})\rangle$$

- Berry connection

$$|D_\mu\Psi\rangle \equiv |\partial_\mu\Psi\rangle - i\mathcal{A}_\mu|\Psi\rangle$$

- covariant derivative

significance of covariant derivative:

$$|\Psi(\boldsymbol{g})\rangle \rightarrow e^{i\chi(\boldsymbol{g})}|\Psi(\boldsymbol{g})\rangle$$

$$|D_\mu\Psi(\boldsymbol{g})\rangle \rightarrow e^{i\chi(\boldsymbol{g})}|D_\mu\Psi(\boldsymbol{g})\rangle$$

Transform the same way with a gauge change

$$\langle\Psi(\boldsymbol{g})|D_\mu\Psi(\boldsymbol{g})\rangle = 0$$

gauge-invariant relation (parallel transport)

- after a gauge transformation:

$$\mathcal{A}_\mu \rightarrow \mathcal{A}_\mu + \partial_\mu \chi(\boldsymbol{g})$$

not gauge invariant

- The metric and Berry curvature <u>are</u> gauge-invariant

$$\mathcal{G}_{\mu\nu} = \mathrm{Re.}(\langle \partial_\mu \Psi | \partial_\nu \Psi \rangle) - \mathcal{A}_\mu \mathcal{A}_\nu$$

$$\mathcal{F}_{\mu\nu} = \partial_\mu \mathcal{A}_\nu - \partial_\nu \mathcal{A}_\mu$$

- We can also make a GR-like covariant tensor formulation by using the metric to obtain the <u>Christoffel connection</u>:

- $$D_\mu \mathcal{V}_\nu \equiv \partial_\mu \mathcal{V}_\nu - \Gamma^\sigma_{\mu\nu} \mathcal{V}_\sigma$$

$$\mathcal{F}_{\mu\nu} = D_\mu \mathcal{A}_\nu - D_\nu \mathcal{A}_\mu$$

unchanged
(antisymmetric)

Unitary case:
Berry phase and Chern invariant:

- For a closed path Γ on the manifold:

$$e^{i\phi(\Gamma)} = \exp i \oint_{\Gamma} \mathcal{A}_\mu dg^\mu$$

geometrical U(1)
Berry phase factor

- For a closed 2-surface Σ on the manifold:

$$\frac{1}{2\pi}\int_{\Sigma} dg^\mu \wedge dg^\nu \mathcal{F}_{\mu\nu} = C_1(\Sigma)$$

topological
(1st) Chern class
integer invariant

(These are the analogs of the Bohm-Aharonov phase and the Dirac monopole quantization)

Orthogonal case:

- Vanishing Berry curvature

$$\mathcal{F}_{\mu\nu} = 0$$

- Berry phase factor:

$$\eta(\Gamma) = \exp i \oint_{\Gamma} \mathcal{A}_{\mu} dg^{\mu} = \pm 1$$

topological Z(2)
Berry phase factor

Symplectic case:

- As above, plus Chern invariant

$$\frac{1}{24\pi^2} \int_{\mathcal{M}_4} dg^{\mu} \wedge dg^{\nu} \wedge dg^{\sigma} \wedge dg^{\tau} \rho_{\mu\nu\sigma\tau} = C_2(\mathcal{M}_4)$$

topological
(2nd) Chern class
integer invariant

$$\rho_{\mu\nu\sigma\tau} \equiv \mathcal{F}^a_{\mu\nu}\mathcal{F}^a_{\sigma\tau} + \mathcal{F}^a_{\mu\tau}\mathcal{F}^a_{\nu\sigma} + \mathcal{F}^a_{\mu\sigma}\mathcal{F}^a_{\tau\nu}$$

integral over
closed 4-d surface

(O(3) vector dot product)

2D manifolds.

- There is only one independent 2-form (volume element) of an (orientable) 2-d manifold; all others can be related to it. Various choices are possible.

$$\mathcal{F}_{\mu\nu}(\boldsymbol{g}) = \mathcal{F}(\boldsymbol{g})(\det \mathcal{G}(\boldsymbol{g}))^{1/2}\epsilon_{\mu\nu}$$ antisymmetric symbol

- since $\mathcal{G}_{\mu\nu} \pm i\mathcal{F}_{\mu\nu}$ is positive Hermitian, $\mathcal{F}$ is a dimensionless pseudoscalar with the bounds

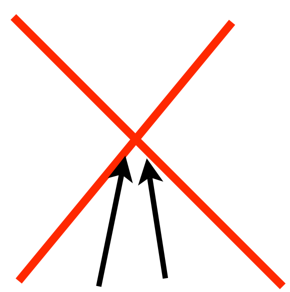
$$0 \le (\mathcal{F}(\boldsymbol{g}))^2 \le 1$$ (unitary case)

$$0 \le \mathcal{F}^a(\boldsymbol{g})\mathcal{F}^a(\boldsymbol{g}) \le 1$$ (symplectic case)

In general

$$\mathcal{G}_{\mu\lambda}\mathcal{G}^{\lambda\nu} = \delta^{\nu}_{\mu} \qquad \mathcal{G}_{\mu\nu} \geq \mathcal{G}^{\kappa\lambda}\mathcal{F}_{\mu\kappa}\mathcal{F}_{\nu\lambda}$$

- If the Berry curvature diverges at some point, so does the Riemann metric.
- These divergences are associated with "Dirac points" where bands touch linearly - like "wormholes" in GR though which quantized magnetic flux passes.



distance 1 between "close" points

History:

- The Riemann metric structure was explored (in the mathematical context of coherent states) by Provost and Vallee (1980) who noted in passing that there was also an antisymmetric part that might also be worth studying .....(now known as Berry curvature (!)) Not much tangible physics has emerged from the metric, until recently what appears to be developing into a fundamental characterization of localization lengths in band insulators has been formulated (Marzani and Vanderbilt, (1997) Resta and Sorella (1999), Souza)
- The Berry curvature, following from the Berry phase (1984), the TKNN (1984) treatment of the QHE, followed by Simon's (1984) mathematical explanation continues to play a major role in modern physics.

Application to Bloch states

$$\psi_{\boldsymbol{R},i}(\boldsymbol{k}) = e^{i\boldsymbol{k}\cdot(\boldsymbol{R}+\boldsymbol{r}_i)}u_i(\boldsymbol{k})$$

- amplitude for a particle to be on i'th site at position $\boldsymbol{R}$ + $\boldsymbol{r}_i$ in unit cell $\boldsymbol{R}$. Note that the Bloch factor depends on the assumed relative location of site i in the unit cell.

changing the set $\boldsymbol{r}_i$ changes the quantum metric

- Manifold is the Brillouin zone $\boldsymbol{k} \bmod \boldsymbol{G}$. Berry connection is

$$\mathcal{A}^a(\boldsymbol{k}) = -i\sum_i u_i^*(\boldsymbol{k})\nabla_k^a u_i(\boldsymbol{k})$$

- "mean position of particle relative to unit cell" $r^a = -i\nabla_k^a - \mathcal{A}^a(\boldsymbol{k})$

$$[r^a, r^b] = i\mathcal{F}^{ab}(\boldsymbol{k})$$

non-commuting coordinates!

- What physical properties are influenced by the “quantum geometry” of the Bloch states at the Fermi level?
- NOT static ground state properties; only properties that involve acceleration of particles at the Fermi surface by applied uniform electric fields, chemical potential and thermal gradients, etc.
- unaccelerated particles are not influenced by these effects, but they can have a profound effect on transport.

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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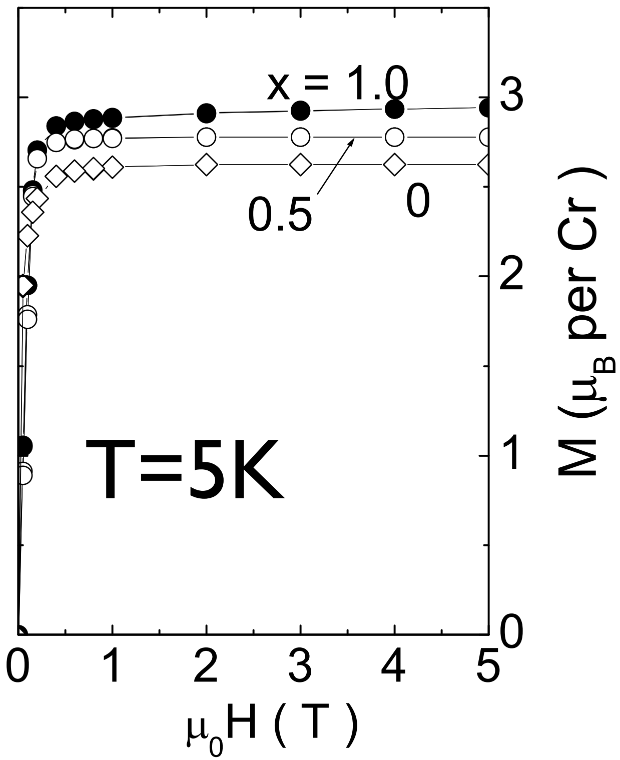
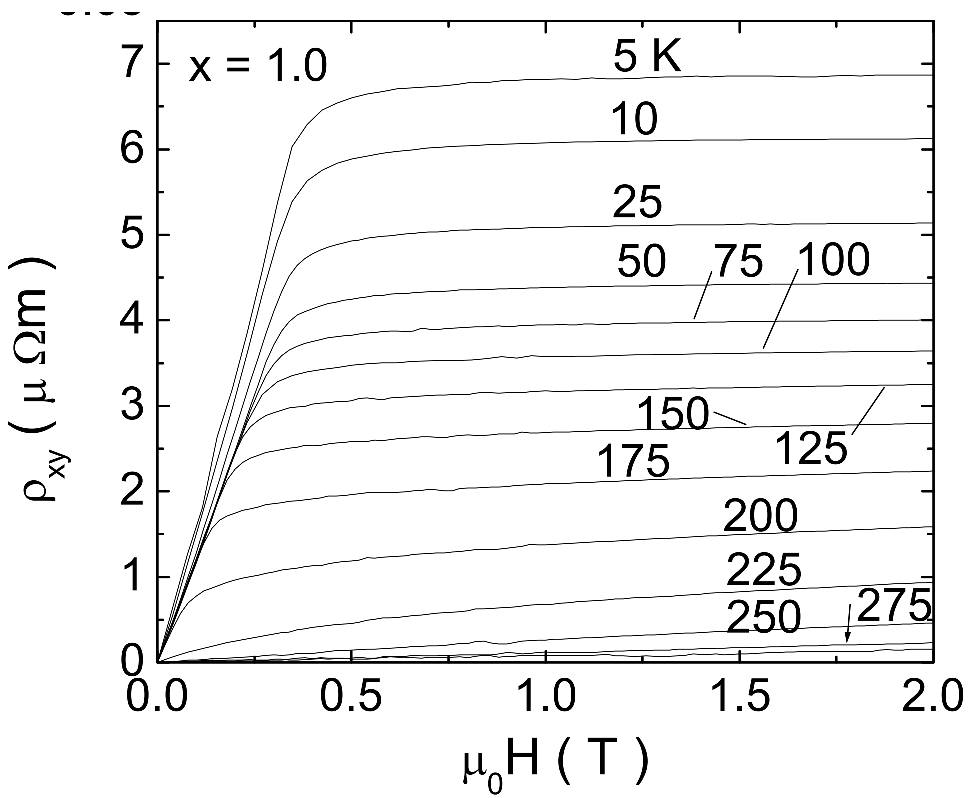




example of a very large AHE

- 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")

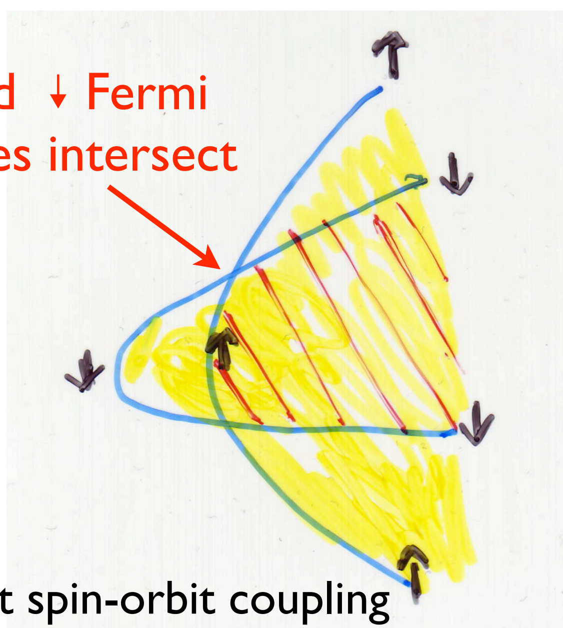
In different regimes of temperature and purity, either of these mechanisms may dominate. In many systems, the controversial Karplus-Luttinger mechanism dominates.

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.

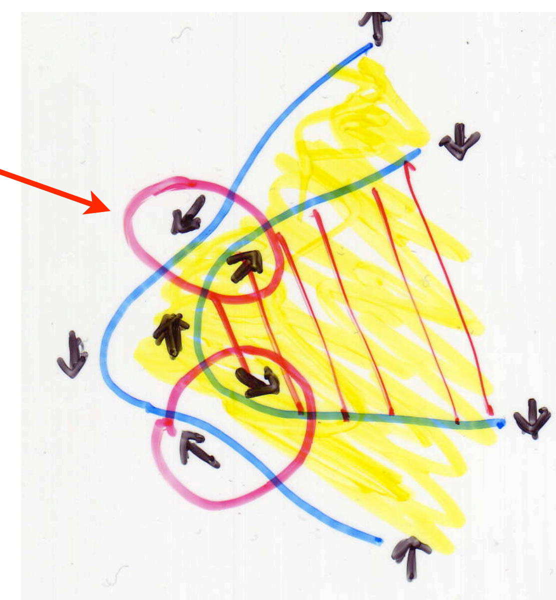
- In this picture, the majority and minority spin Fermi surfaces are independent, and can intersect:

↑ and ↓ Fermi surfaces intersect

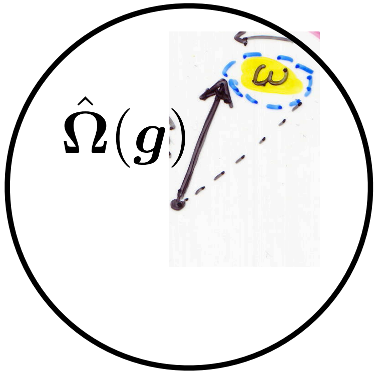


without spin-orbit coupling

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)

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

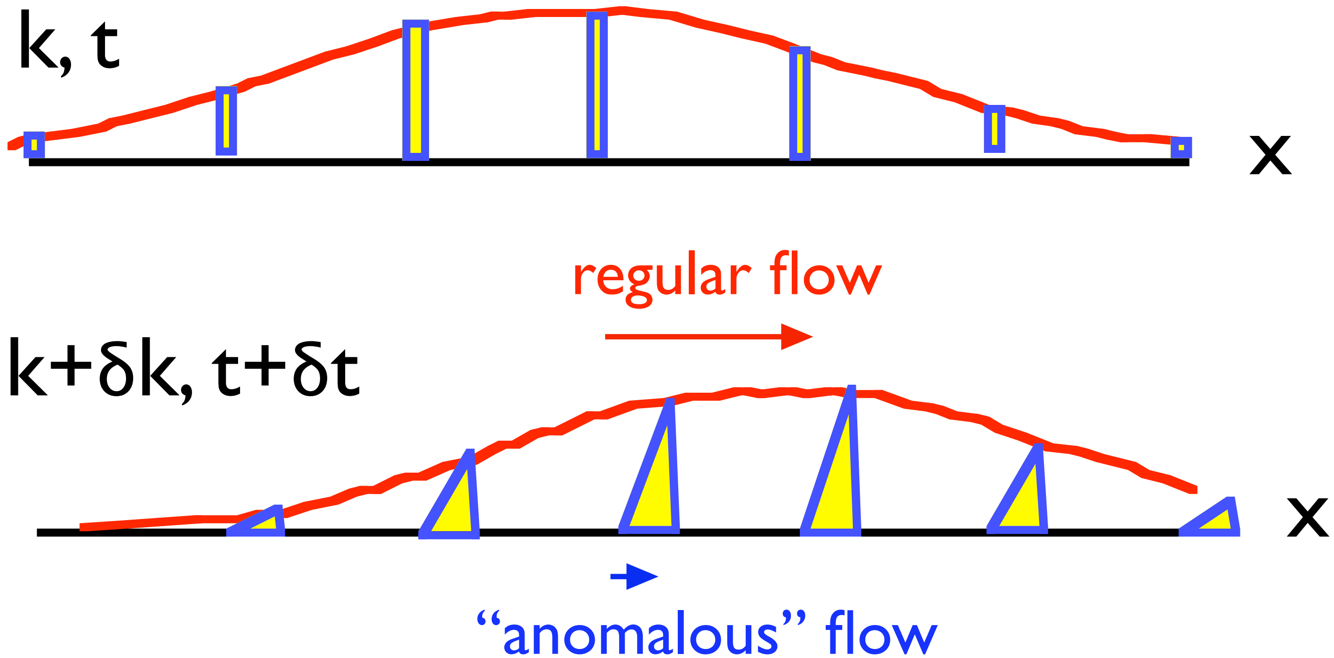
$$H(\boldsymbol{r}, \boldsymbol{k}) = \varepsilon_n(\boldsymbol{k}) + V(\boldsymbol{r})$$

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).

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

- 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 $t_2e^{i\varphi}$, alternating onsite potential M.)

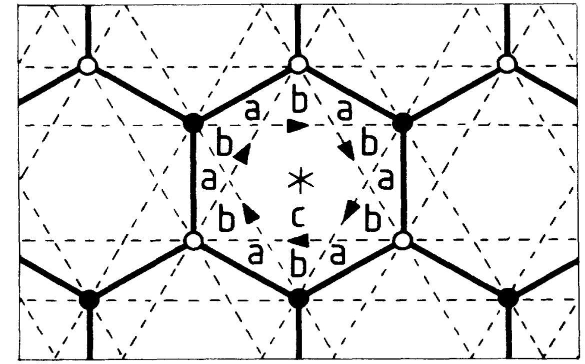


FIG. 1. The honeycomb-net model ("2D graphite") showing nearest-neighbor bonds (solid lines) and second-neighbor bonds (dashed lines). Open and solid points, respectively, mark the A and B sublattice sites. The Wigner-Seitz unit cell is conveniently centered on the point of sixfold rotation symmetry (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.

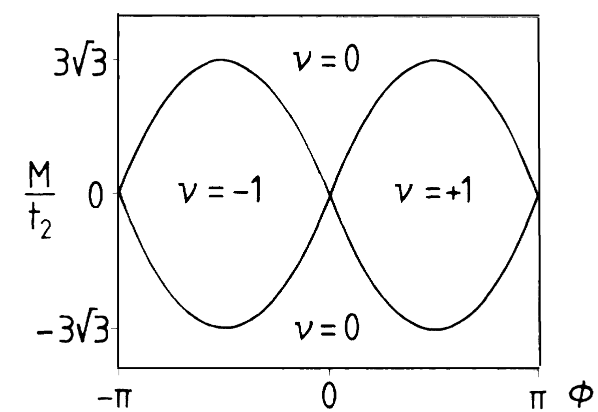
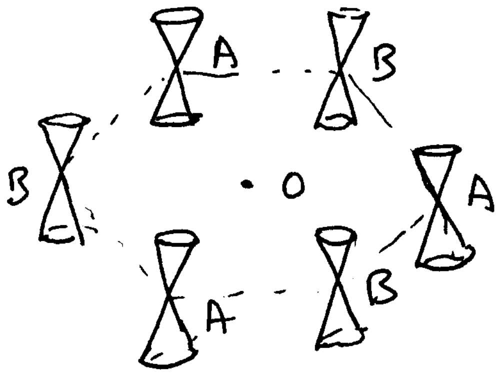
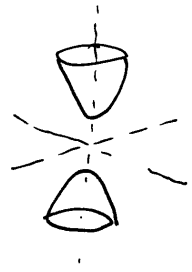


FIG. 2. Phase diagram of the spinless electron model with $|t_2/t_1| < \frac{1}{3}$. Zero-field quantum Hall effect phases ($\nu = \pm 1$, where $\sigma^{xy} = \nu e^2/h$) occur if $|M/t_2| < 3\sqrt{3}|\sin\phi|$. This figure assumes that t_2 is positive; if it is negative, ν changes sign. At the phase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

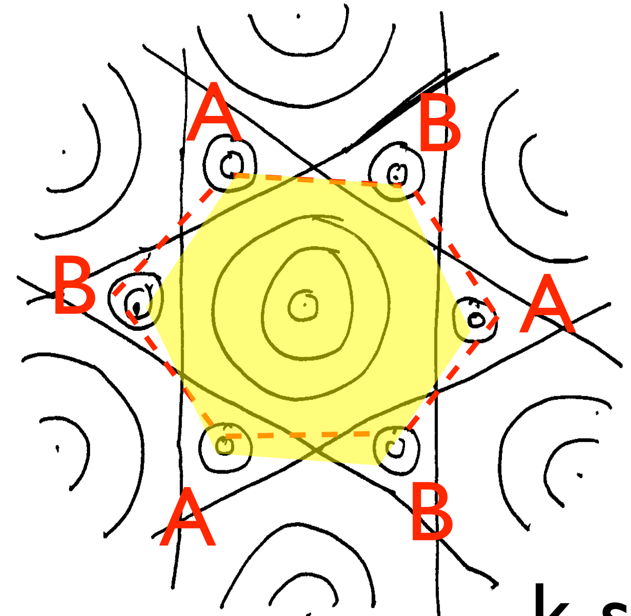
2D “graphene” bandstructure



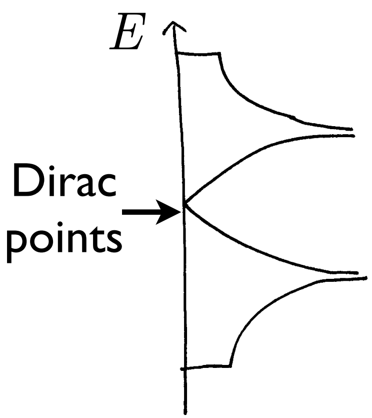
two distinct “Dirac points” (at corners of hexagonal Brillouin zone)



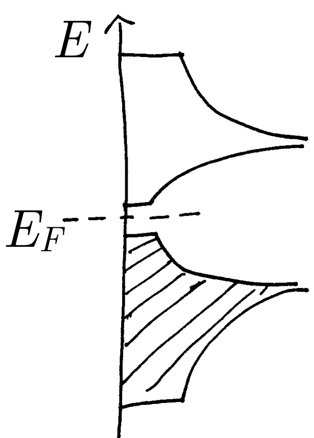
Breaking either inversion (I) or time-reversal (T) symmetry opens a “mass gap” at Dirac points.)



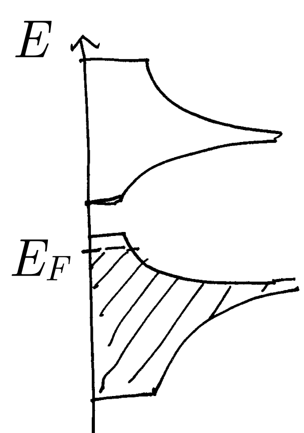
k-space



density of states (massless)



massive case (bulk insulator)



massive case (bulk metal)

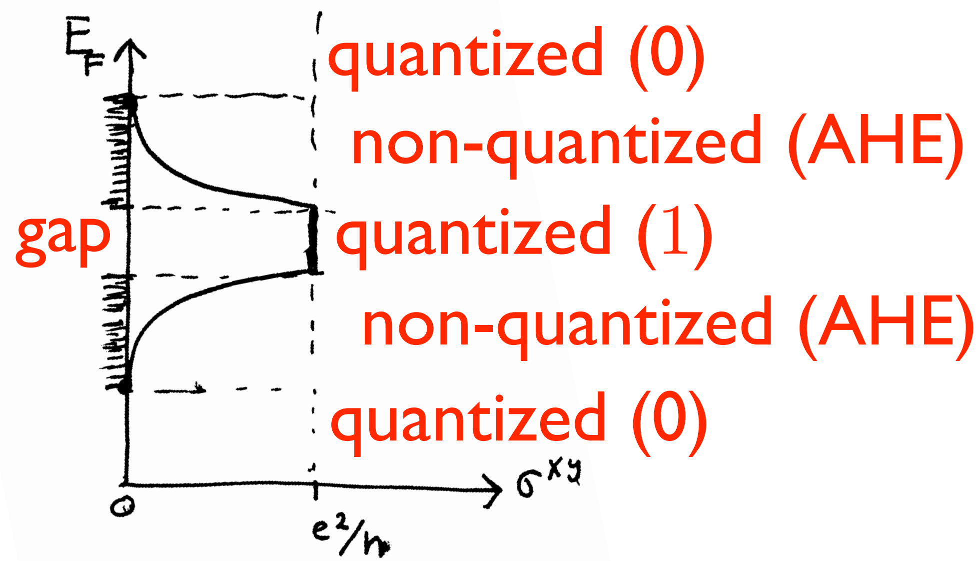
Break only T: $m_A = m_B$

<u>same sign</u> Berry curvature near A and B points

Break only I: $m_A = -m_B$

<u>opposite sign</u> Berry curvature near A and B points

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

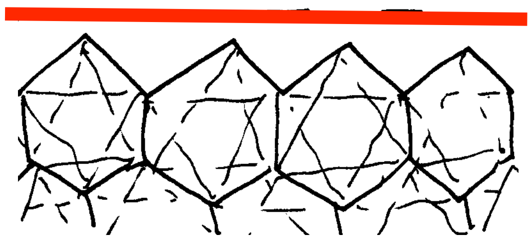


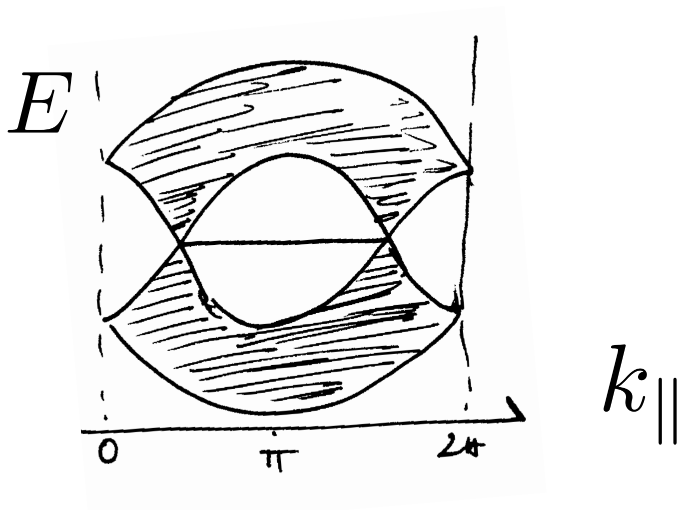
Graphene model with second neighbor hopping is very useful!

- 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)

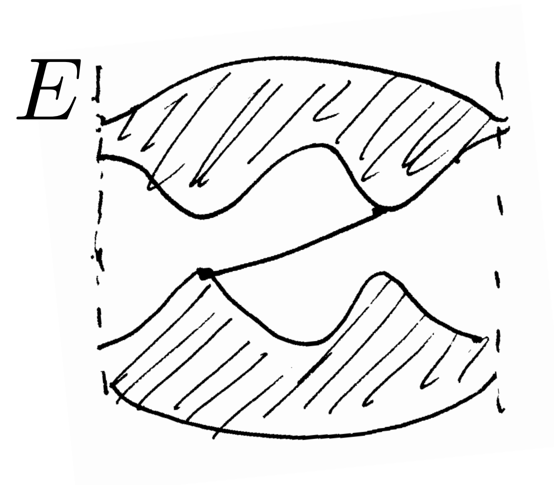
- graphene edge states (zigzag edge)

edge

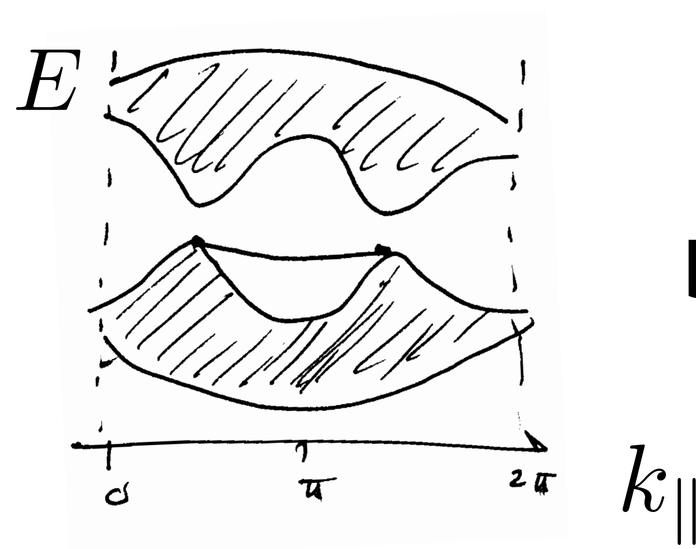




gapless case



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.**

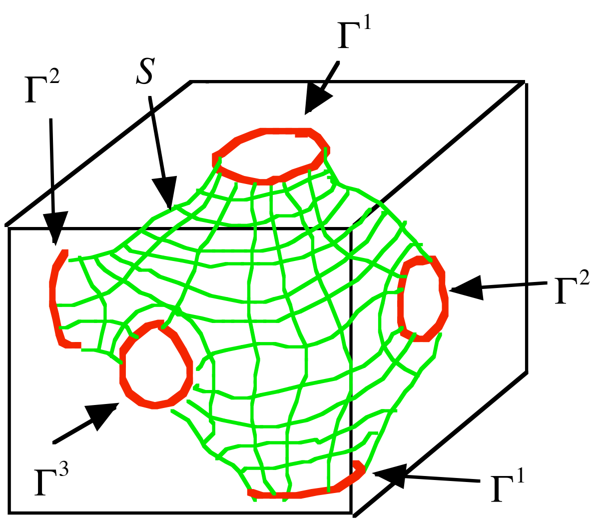
- Intersections with the Brillouin-zone boundary need to be taken into account.

"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

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Phys. Rev. Lett. 92, 037204 (2004)

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 **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.

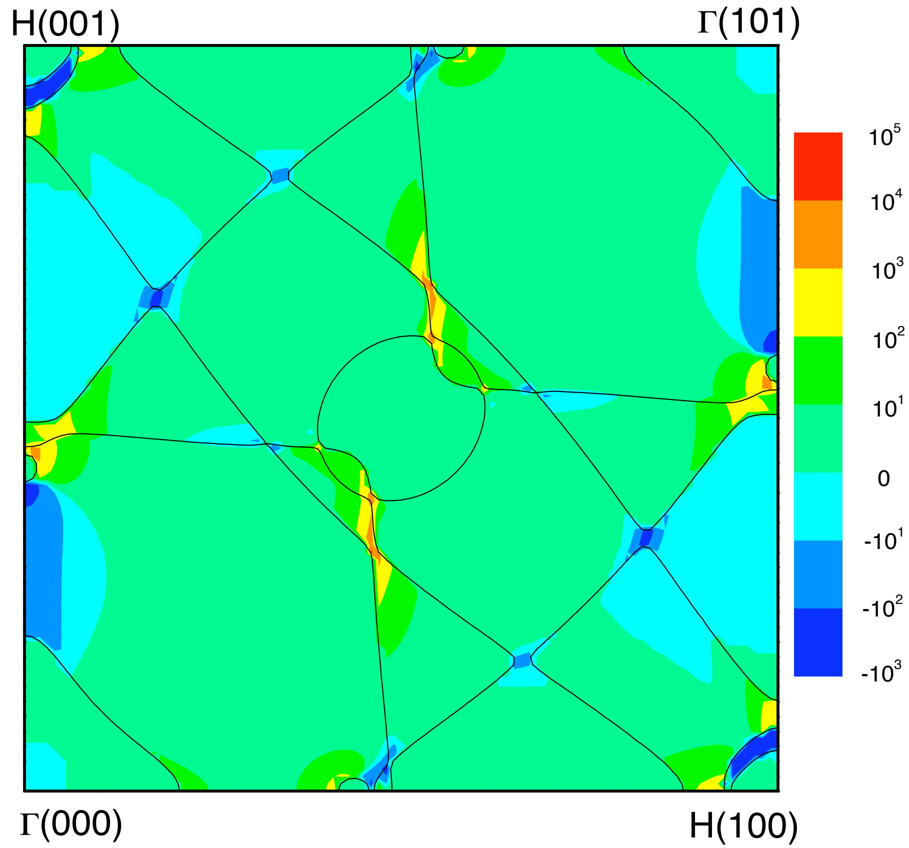
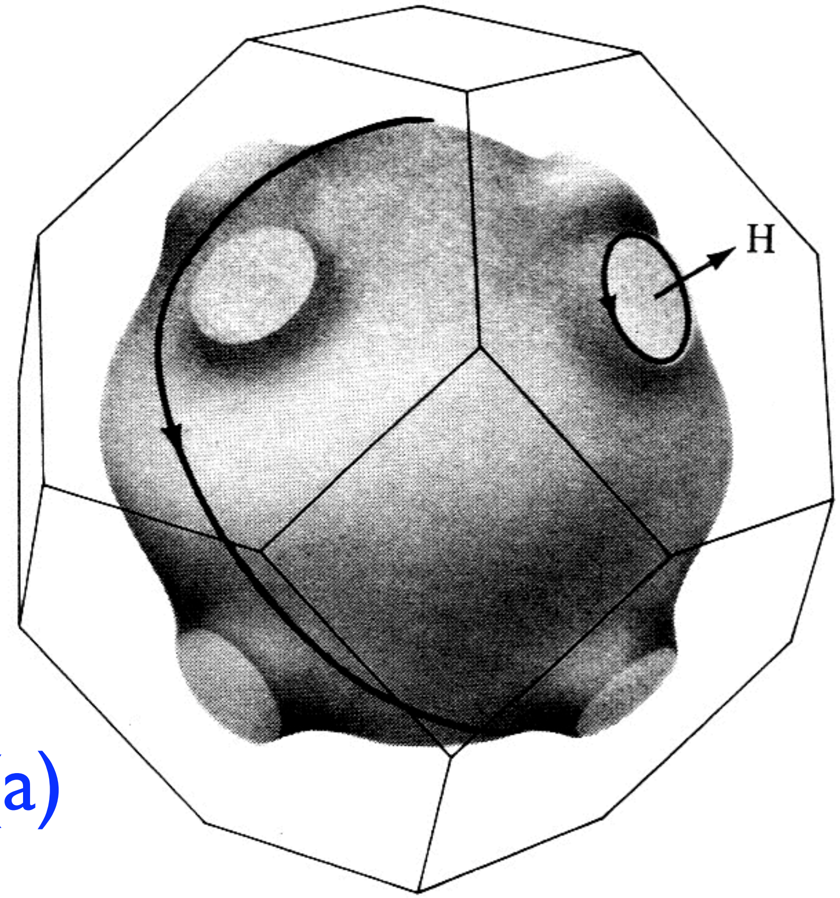


FIG. 4: (010) plane Fermi-surface (solid lines) and Berry curvature $-\Omega^z(\mathbf{k})$ (color map). $-\Omega_z$ is in atomic units.

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.

- The new Fermi-surface Berry curvature formula suggests a different - intrinsic - way to think about Fermi surface geometry in Fermi liquid theory.....

Fermi surface of a noble metal (silver):

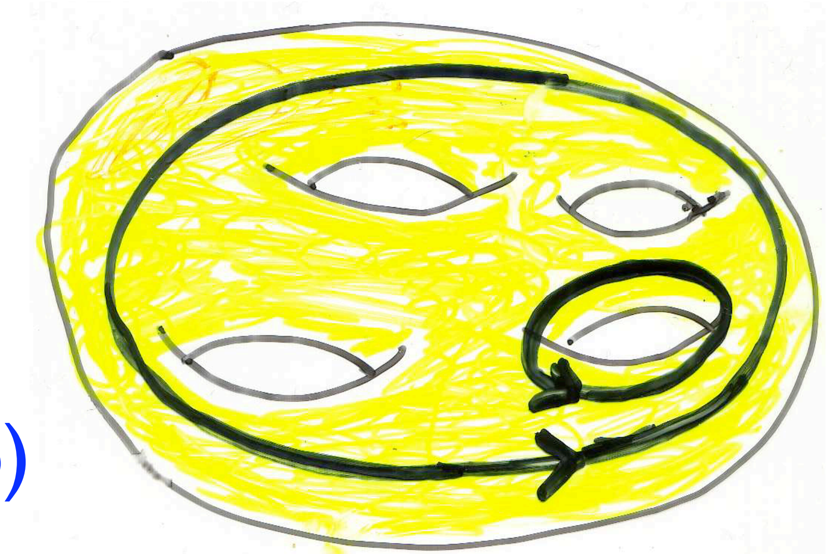


(a)

conventional view as a surface in the Brillouin zone, periodically repeated in k-space

De Haas-Van Alpen effect allows extremal cross-sections to be experimentally determined

(b)



Abstract view of the same surface (and orbits) as a compact manifold of quasiparticle states

(with genus g = 4,

“open-orbit dimension” d^G = 3).

Dimension of Bravais lattice of reciprocal lattice vectors G corresponding to k-space displacements associated with periodic open orbits on the manifold.

Ingredients of Fermi-liquid theory on a Fermi-surface manifold

k-space geometry

$\boldsymbol{k}_F(\boldsymbol{s})$ Fermi vector

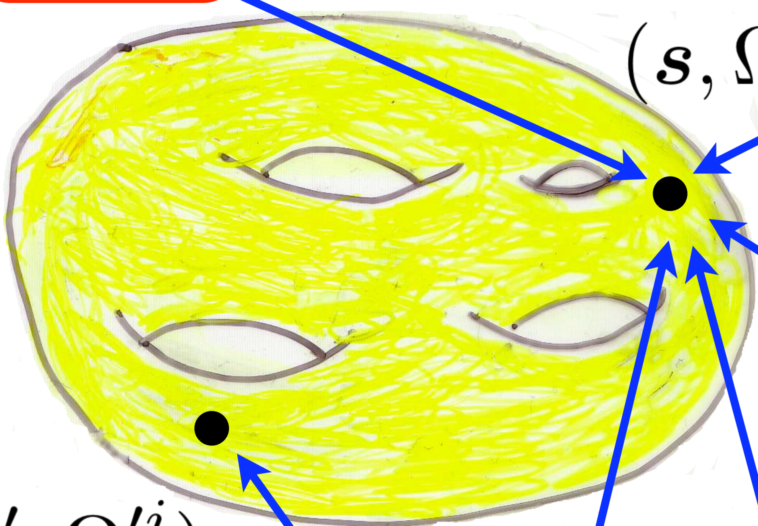
$\hat{\boldsymbol{n}}_F(\boldsymbol{s})$ direction of Fermi velocity

k-space metric
$\mathcal{G}^F_{\mu\nu}(\boldsymbol{s}) \equiv \partial_\mu \boldsymbol{k}_F \cdot \partial_\nu \boldsymbol{k}_F$

kinematic parameters

$\ell(\boldsymbol{s})$ inelastic mean free path

$Z(\boldsymbol{s})$ renormalization factor



Hilbert-space geometry

$\mathcal{G}^H_{\mu\nu}(\boldsymbol{s})$ Hilbert-space metric

$\mathcal{A}_\mu(\boldsymbol{s})\ \mathcal{A}^i_\mu(\boldsymbol{s})$ Berry gauge fields:

Z(2) + SO(3) $g_s = 2$

U(1) $g_s = 1$

Fermi surface spin degeneracy

NEW

quasiparticle energy parameters

$f(\boldsymbol{s}, \boldsymbol{s}')\quad f^{ij}(\boldsymbol{s}, \boldsymbol{s}')$

Landau functions
coupling pairs of quasiparticle states

$v_F(\boldsymbol{s})$ Fermi speed

$\boldsymbol{\mu}^i(\boldsymbol{s})$ quasiparticle magnetic moment

quasiparticle coordinate:

manifold coordinate (d=2) $\{s^\mu, \mu = 1, 2\}$

$(\boldsymbol{s}, \Omega^i)$

spin coherent-state direction $\{\Omega^i, i = 1, 2, 3\}$

Quasiparticles "live" only on the Fermi surface.

- This leads to a 5-dimensional symplectic (phase space) structure:
  - 3 real space + 2 k-space
  - 2 pairs + 1 "chiral" unpaired real space direction at each point on the Fermi-surface manifold
  - the unpaired direction is the local Fermi velocity direction.

Physical significance of "Hilbert space geometry"

$\mathcal{G}^H_{\mu\nu}(\boldsymbol{s})$ Hilbert-space metric

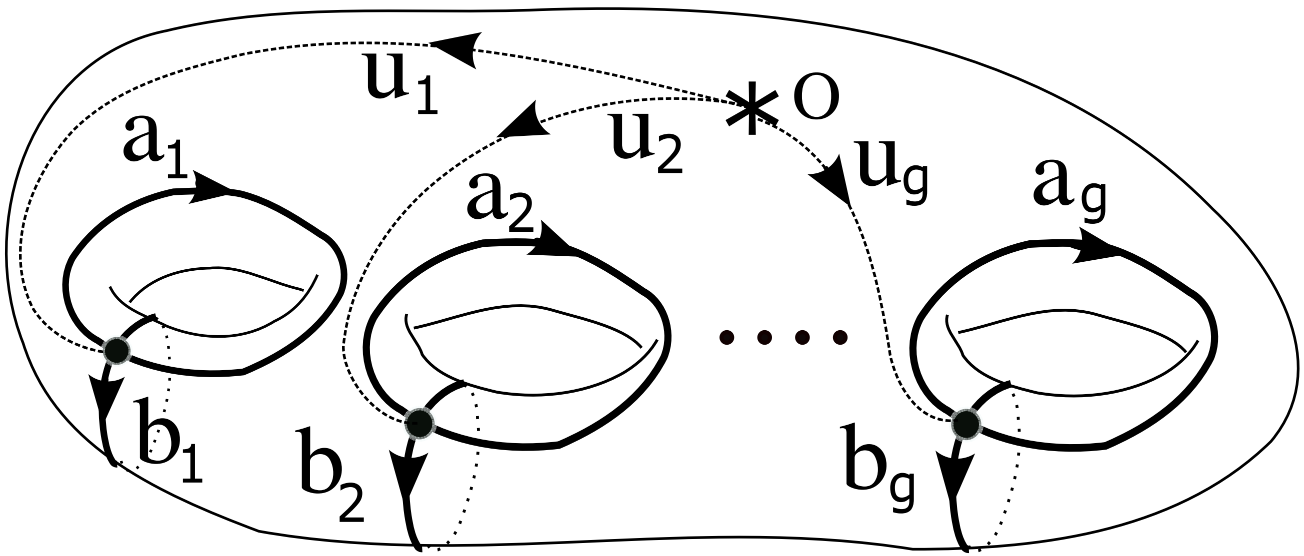
$\mathcal{A}_\mu(\boldsymbol{s})\,\mathcal{A}^i_\mu(\boldsymbol{s})$ Berry gauge fields:

- Z(2) + SO(3) $g_s = 2$ ← if both spatial inversion and time-reversal symmetry are present*
- U(1) $g_s = 1$ ← otherwise*

* assumes spin-orbit coupling

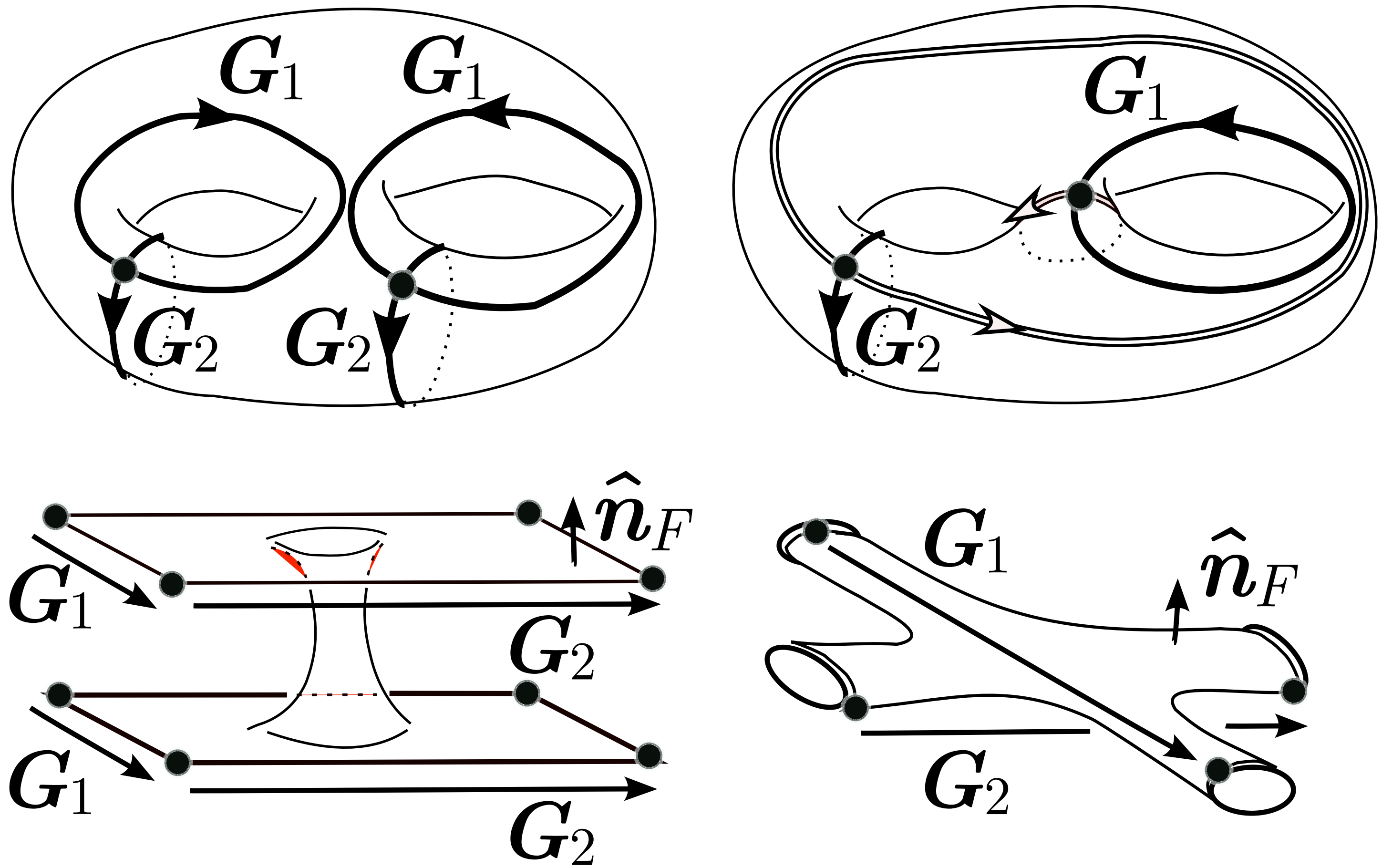
- The Hilbert-space metric and the Berry gauge fields modify the ballistic behavior of quasiparticles which are accelerated by quasi-uniform electromagnetic fields, chemical potential and thermal gradients, strain fields, etc.
- Hilbert space geometric effects are completely omitted in a single-band approximation that also neglects spin-orbit coupling (like a one-band Hubbard model).

“intrinsic” picture of Fermi surface as an abstract 2-manifold



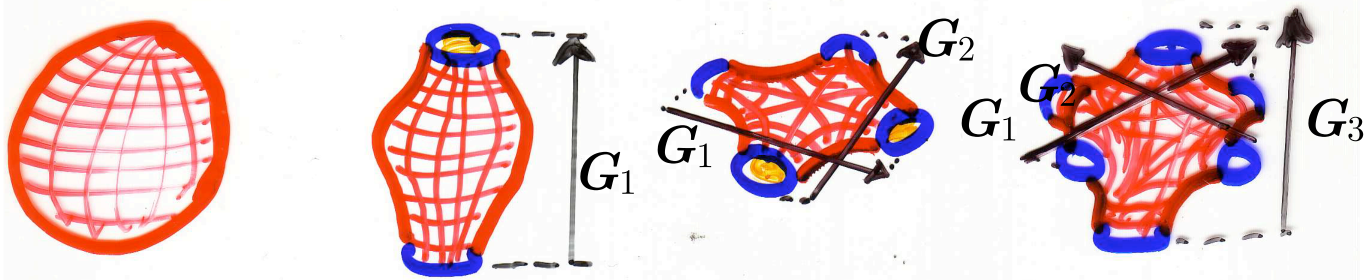
- “homology group” has a basis of G (=genus) pairs of non-trivial paths (that don’t cut the manifold in half). Only members of the same pair intersect. Open orbits (along which $\boldsymbol{k}_F$ increases by a reciprocal lattice vector $\boldsymbol{G}$) are non-trivial.

two different ways to view a genus-2 Fermi surface of “open-orbit dimension” d_G=2

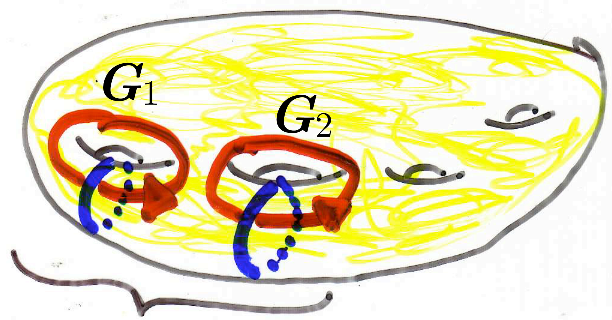


Standard "schema" (homology group) for Fermi surface manifolds:

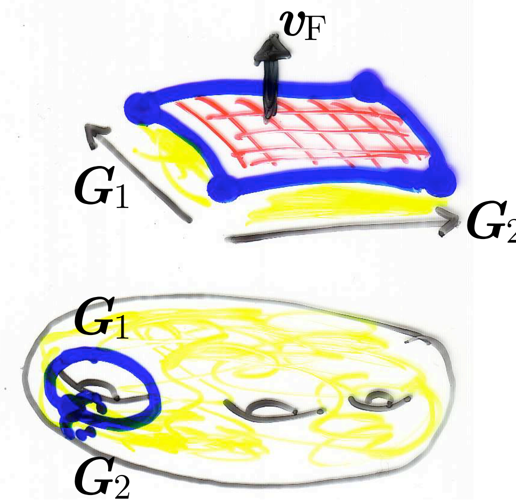
k-space images $d^G=0$ $d^G=1$ $d^G=2$ $d^G=3$



a 2-manifold of genus g has g conjugate pairs of elementary non-trivial closed paths (homology group generators)



$d^G=2$, chiral



normal case:

the first d^G pairs of generators couple a closed-orbit "zone boundary" with an "open orbit"

chiral (quasi-1d) case:

the first pair of generators are both "open orbits" AND "zone boundaries."

d^G =0,1,2, or 3 is the dimension of the Bravais lattice of reciprocal vectors generated by "open orbits". (If chiral quasi-1D Fermi surfaces are present, d^G =0,1,or 2)

- separate dissipationless Hall currents (with their own adiabatic conservation laws) on each distinct manifold (generalizes separate conservation law of each chiral Fermi point in 1D to 3D) . A separate chemical potential can be established on each manifold.

- Fermi surface with non-zero Chern numbers are connected by "wormholes" (Dirac degeneracy points that connect bands; see also discussions of "Fermi points" by Volovik). Charge can be transferred through the "wormhole", so such connected Fermi surfaces must have the same chemical potential.

- Streda formula:(charge density induced by magnetic field is also controlled by the Hall vector $\boldsymbol{K}$):

Streda formula

- the Hall conductance (linear response of transverse electric current density to electric field) also describes linear response of electron density n to magnetic flux density

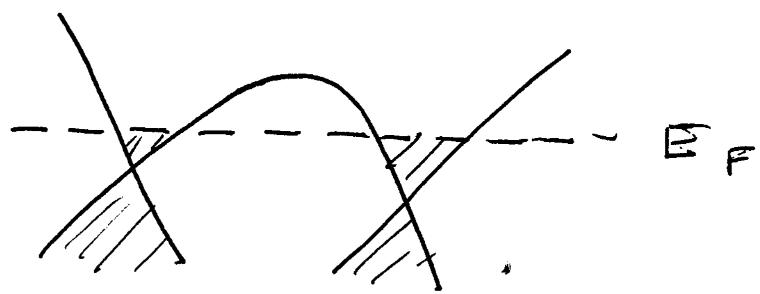
$$\left.\frac{\partial n}{\partial \boldsymbol{B}}\right|_{\mu, T=0} = \frac{e}{h}\frac{\boldsymbol{K}}{2\pi}$$

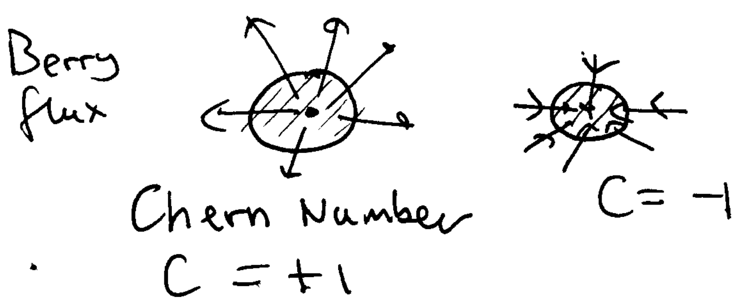
- Xiao, Shi and Niu (2005) note that

Fermi occupation factor

$$n = \int d^3k \left(1 + \epsilon_{abc}\frac{eB^a}{\hbar}\mathcal{F}^{bc}\right) n(\boldsymbol{k})$$

- Fermi surface sheets with non-zero chern number (total Fermi surface Chern number must vanish, but individual pieces can have non-zero Chern number)



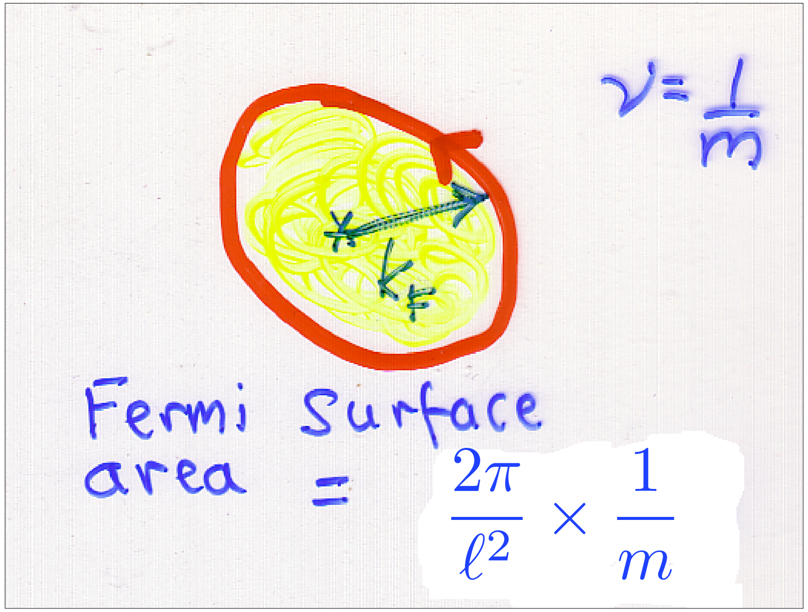


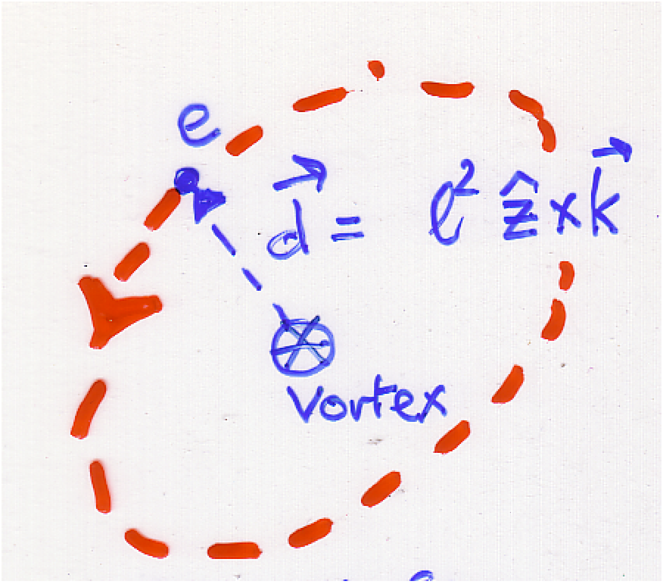
Worm hole!

- As in one dimension, each distinct piece of the Fermi surface has its own “adiabatic conservation law” in the low-T limit, in the absence of large-momentum-transfer scattering processes.
- Pieces of FS with non-zero Chern number only have such a conservation law as a group with zero total Chern number: charge can be “pumped” between them through the “wormhole” that connects them!

Application of formula to composite fermion Fermi surface at $\nu = 1/m$

a composite fermion is modeled as an electron laterally displaced from the center of the m-vortex that is bound to it.





Berry phase for moving composite quasiparticle around Fermi-surface ⇨ Flux enclosed by path of displaced electron around vortex:

$$\boxed{\sigma^{xy}_{\mathrm{AHE}} = \frac{e^2}{h}\frac{1}{m}}$$

independent of Fermi surface shape!

- The Fermi surface formulas for the non-quantized parts of the Hall conductivity are purely "geometrical" (referencing both k-space and Hilbert space geometry)
- Such expressions are so elegant that they "must" be more general than free-electron band theory results!
- This is true: they are like the Luttinger Fermi surface volume result, and can be derived in the interacting system using Ward identities.

An exact formula for the T=0 DC Hall conductivity:

- While the ***Kubo formula*** gives the conductivity tensor as a current-current correlation function, a ***Ward-Takahashi identity*** allows the $\omega \to 0$, $T \to 0$ limit of the (volume-averaged) antisymmetric (Hall) part of the conductivity tensor to be expressed ***completely in terms of the single-electron propagator!***

- The formula is a simple generalization and rearrangement of a 2+1D QED_3 formula obtained by Ishikawa and Matsuyama (Z. Phys C 33, 41 (1986), Nucl. Phys. B **280**, 523 (1987)), and later used in their analysis of possible finite-size

$$G_{ij}(\boldsymbol{k},\omega) = -i\int_{-\infty}^{\infty} dt\, e^{-i\omega t}\langle T_t\{c_{\boldsymbol{k}i}(t), c^\dagger_{\boldsymbol{k}j}(0)\}\rangle \qquad \{c_{\boldsymbol{k}i}, c^\dagger_{\boldsymbol{k}j}\} = \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{ij}$$

exact (interacting) T=0 propagator

(PBC, discretized k)

$$\lim_{\omega,T\to 0}\sigma_H^{ab}(\omega,T) = \frac{e^2}{\hbar}\frac{\epsilon^{abc}}{(2\pi)^2}K_c$$

antisymmetric part of conductivity tensor

$$\boxed{K_a = \lim_{\eta\to 0^+}\frac{\epsilon_{abc}}{2\pi}\int_{BZ} d^3\boldsymbol{k}\int_{-\infty}^{\infty}\frac{d\omega}{2\pi}e^{i\omega\eta}\mathrm{Tr}\left((\nabla_k^b\frac{\partial}{\partial\omega}(\ln\boldsymbol{G}))(\boldsymbol{G}\nabla_k^c\boldsymbol{G}^{-1})\right)}$$

agrees with Kubo for free electrons, but is quite generally ***EXACT*** at T=0 for interacting Bloch electrons with local current conservation (gauge invariance).

$$K_\alpha = \lim_{\eta \to 0^+} \int_{\mathrm{BZ}} d^3\boldsymbol{k} \int_{-\infty}^{\infty} \frac{d\omega}{2\pi} e^{-i\omega\eta} \mathrm{Tr}\left((\nabla_k^b \frac{\partial}{\partial \omega} (\ln \boldsymbol{G}))(\boldsymbol{G}\nabla^c \boldsymbol{G}^{-1}) \right)$$

- Simple manipulations now recover the result unchanged from the free-electron case.
- The fundamental Luttinger (1961) theorem relating the non-quantized part of the electron density to the Fermi surface volume now has a "partner". (in fact, its derivative w.r.t. B)