BERRY CURVATURE ON THE FERMI-SURFACE:

Anomalous Hall Effect in metallic Ferromagnets as a Topological Fermi-Liquid property.

- Cond-mat/0408417 (PRL, october 8, to appear)

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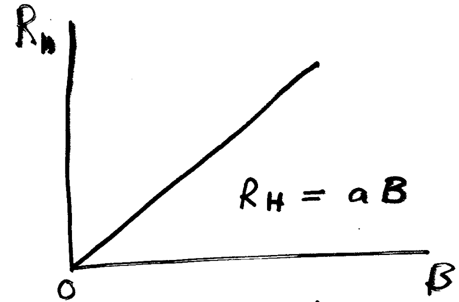
- A Fundamental extension of Landau's Fermi liquid Theory to include Berry phases of QUASIPARTICLES in clean metals with broken Time reversal and/or Inversion symmetry.

- Reveals a rich new 'topological physics' not previously recognized in FLT.

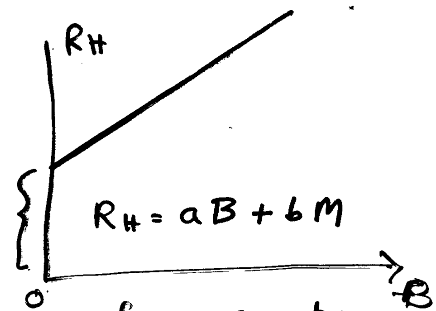
- experimentally realized in recent AHE measurements of low T clean limit of Ferromagnetic metals. Integrates old Karplus-Luttinger formula into FLT

* NSF-MRSEC DMR 02-13706

ANOMALOUS HALL EFFECT (AHE



normal metal



ferromagnetic metal (BROKEN TIME-REVERSAL symmetry)

- metals with Broken time-reversal symmetry, BUT with $B = 0$ can still exhibit a Hall effect

  = "ANOMALOUS HALL EFFECT"

- Karplus and Luttinger (1954) looked at

CONTROVERSIAL! $\sigma^{xy} = \dfrac{\rho^{xy}}{\rho^{xx} + \rho^{xy}}$

→ and found it had an "intrinsic component" That survived in The "clean limit" where The scattering time $\tau \to \infty$.

- Recent experiments
  Fang et al. Science 302, 92 (2003)
  Lee et al. Science 303, 1647 (2004)
  Show The intrinsic contribution dominates in The low T clean limit.

- Recent reinterpretations of Karplus-Luttinger (Kubo) formula identify their "anomalous velocity" with ~~the~~ $\boxed{\text{Berry Curvature in k-space of the Bloch states}}$

Berry Correction to semiclassical dynamics:
(M. Marder, 1999; Sundaram + Niu, 1999).

$$\boxed{\begin{aligned} \hbar \frac{dk_a}{dt} &= e E_a + e F_{ab} \frac{dx^b}{dt} \\ \frac{dx^a}{dt} &= \underbrace{\frac{1}{\hbar} \nabla_k^a \mathcal{E}_n(k)}_{\text{GROUP VELOCITY}} + \underbrace{\mathcal{F}_n^{ab}(k) \frac{dk_b}{dt}}_{\text{ANOMALOUS VELOCITY}} \end{aligned}}$$

Lorentz force

k-space dual of Lorentz force

$$F_{ab} = \nabla_a A_b(x) - \nabla_b A_a(x) = \epsilon_{abc} B^c(x)$$

$$\mathcal{F}_n^{ab}(k) = \nabla_k^a a_n^b(k) - \nabla_k^b a_n^a(k)$$

$A_a(x)$ = electromagnetic vector potential

$$a_n^a(k) = \langle \psi_n(k) | -i \nabla_k^a | \psi_n(k) \rangle$$

"Berry vector potential" in k-space

band index

derivative w.r.t. Bloch vector
($\approx$ periodic part of x^a!)

Bloch vector

- Bloch states

$$\psi_n(k) = e^{i\phi_n(k)}\, e^{i\vec{k}\cdot\vec{x}}\, u_n(k,x)$$

arbitrary phase convention

Bloch factor

k and n-dependent periodic part.

- The Berry "vector potential" $a_n^a(\vec{k})$ is determined by the variation of $u_n(k,x)$ with $\vec{k}$

$$a_n^a(k) = -i \frac{\int_{\text{unit cell}} d^3x \; u_n^*(k,x)\, \nabla_k^a u_n(k,x)}{\int_{\text{unit cell}} d^3x \; u_n^*(k,x)\, u_n(k,x)}$$

- if $\phi_n(k) \longrightarrow \phi_n(k) + \chi_n(k)$

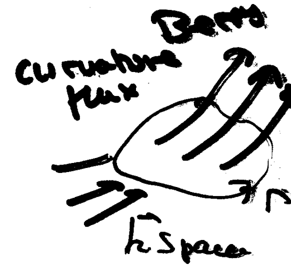
$$a_n^a(k) \longrightarrow a_n^a(k) + \nabla_k^a \chi_n(k)$$

- $F_n^{ab}(k) = \nabla_k^a a_n^b(k) - \nabla_k^b a_n^a(k)$

is unchanged ("Berry-gauge" invariant)

antisymmetric "Berry curvature" induced by $\psi_n(k)$ in k-space.

Adiabatic evolution of the wavefunction around a closed path Γ in k-space



$$e^{i\phi_{Berry}} = \exp i \oint_\Gamma \mathcal{A}^a_n(k)\, dk_a$$

ϕ_{Berry} is ambiguous up to multiples of 2π

"Berry flux quantum" $= 2\pi$

k-space analog of realspace:

$$e^{i \oint_\Gamma \frac{e}{\hbar} \vec{A} \cdot d\vec{\ell}} = e^{i \Phi_{\text{Bohm-aharonov}}}$$

magnetic flux quantum $= 2\pi \hbar/e$

- Inversion symmetry $\vec{x} \to -\vec{x}$

$$F_n^{ab}(\vec{k}) \to F_n^{ab}(-\vec{k}) \qquad \text{even}$$

- Time-reversal symmetry:

$$F_n^{ab}(k) = -F_n^{ab}(k) \qquad \text{odd}$$

- If both are unbroken, (usual case in textbooks)

$$F_n^{ab}(k) = 0$$

NO <u>BERRY CURVATURE</u> IN k-space.

$n_n(k)$ = Fermi occupation factor.

$$J_e^a = \frac{e}{\hbar}\frac{1}{N\Omega}\sum_{kn}\left(\underbrace{\nabla_k^a \mathcal{E}_n(k)\,\delta n_n(k)}_{\text{ohmic current}} + \underbrace{F_n^{ab}(k)\, n_n^0(k\mu)\, E_b}_{\text{intrinsic current}}\right)$$

$n_n^0(k,\mu)$ = ground state occupations

$\delta n_n(k,\mu)$ = non-equilibrium change, $\propto \vec{E}$ induced by electric field

The Karplus - Luttinger "Intrinsic" Hall conductivity, :

$$\sigma_0^{ab}(\mu) = \frac{e^2}{\hbar} \underbrace{\frac{1}{\Omega}}_{\text{Volume of unit cell}} \underbrace{\sum_n}_{\text{Sum over bands}} \underbrace{\int_{BZ} \frac{d^3k}{(2\pi)^3}}_{\text{Integral over Brillouin zone}} \underbrace{F_n^{ab}(k)}_{\text{Berry curvature}} n_n^0(k,\mu)$$

Volume of unit cell

Sum over bands

Integral over Brillouin zone

Berry curvature (antisymmetric tensor) in k-space of band n

equilibrium (Ground State) occupation function at chemical potential μ

σ_0^{ab} VANISHES UNLESS TIME-REVERSAL symmetry is broken

NOTE: This is for non-interacting band electrons:

$n_n^0(k,\mu) \equiv \Theta(\mu - \varepsilon_n(k))$:

all occupied single particle states are apparently involved!

$\varepsilon_n(k)$ and $F_n^{ab}(k)$ are the products of the Band Structure calculators "black art" (NOT IN SPIRIT OF LANDAU!)

The Karplus-Luttinger formula involves properties of single electron states far below the Fermi level of the metal.

But... in real (Fermi liquid) metals properties of "single-particle states" not at the Fermi surface are a figment of a band-structure calculator's imagination, (and "single particle states" at the Fermi level become quasi particle states)

MY NEW RESULT: (cond-mat/0408417, PRL to appear Oct 8)

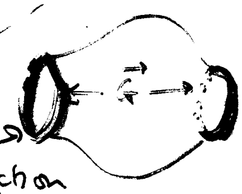
- $\sigma_0^{ab}(\mu) = \frac{e^2}{(2\pi)^2\hbar} \epsilon^{abc} K_c(\mu)$
- $\vec{K}_c(\mu)$ is dimensionally a reciprocal vector.
- up to reciprocal lattice vectors $\vec{G}$, $\vec{K}_c(\mu)$ is completely determined by Berry phases of (quasi particles) ON the Fermi surface
- $\vec{G}$ represents a 3D integer quantum Hall effect.

Berry curvature
on FS

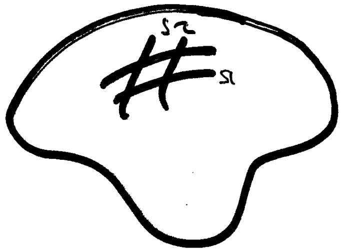
Note: invariant under redefinition of primitive BZ in k-space because of this term.

$$\vec{K}(\mu) = \frac{1}{2\pi}\sum_{S_\alpha}\int ds^\mu \wedge ds^\nu F_{\mu\nu}(\underline{s})\,\vec{k}_F(\underline{s}) + \sum_{i} \frac{\phi_{\alpha i}}{2\pi}\vec{G}_{\alpha i}$$

Berry phase around intersection of FS with BZB



Intersection with Brillouin zone boundary



$\vec{k}_F(s_1, s_2)$ is a 2D parametrization of the Fermi surface sheet α.

I'll explain this formula later...

- Note the Streda-type relation, for the response to a uniform <u>magnetic</u> field:

electric charge density: $$\left.\frac{\partial \rho_e}{\partial \vec{B}}\right)_\mu = \frac{e^2}{(2\pi)^2\hbar}\vec{K}(\mu)$$

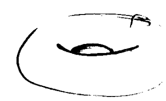
$$\sigma_0^{ab}(\mu) = \frac{e^2}{(2\pi)^2\hbar}\epsilon^{abc}K_c(\mu) = \left.\frac{\partial J_e^a}{\partial E_b}\right)_\mu$$

Continuity equation + Faraday law

2D Band structure invariant
= Chern number (First Chern class)

$$\frac{1}{2\pi}\int_{BZ(2D)} d^2k \; F_n^{xy}(k) = \mathbb{C}_n \quad \text{, integer}$$

BZ (2D)
(= TORUS)



In general — Berry curvature

$$\frac{1}{2\pi}\int_{S'} ds^\mu \wedge ds^\nu \; F_{\mu\nu}(\underline{s}) = \mathbb{C}(S')$$

integer

for **any** compact closed oriented manifold

$$F_{\mu\nu} = \partial_\mu A_\nu - \partial_\nu A_\mu$$

$$e^{i\Phi_\Gamma} = \exp i \int_\Gamma ds^\mu A_\mu(s)$$

Berry phase — Γ closed loop

3D Band invariant

$$\frac{1}{(2\pi)}\int_{BZ(3D)} d^3k \; F_n^{ab}(k) = \epsilon^{abc}(G_n)_c$$

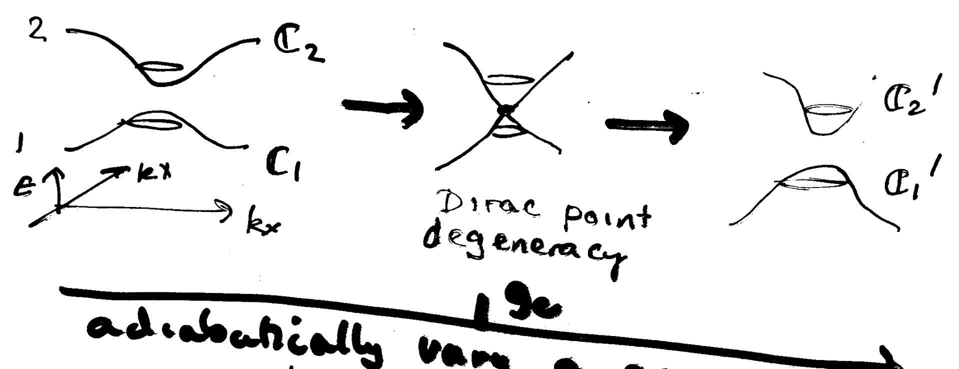
$\vec{G}_n$ = A RECIPROCAL VECTOR

$= \mathbb{C}_n \; \vec{G}_n^c$ ← primitive reciprocal vector (indexes a family of Lattice planes)

integer Chern number (per lattice plane)

How does Chern number of bands Change?

(← 2D)



$\mathbb{C}_2' = \mathbb{C}_2 + n$ ← integer

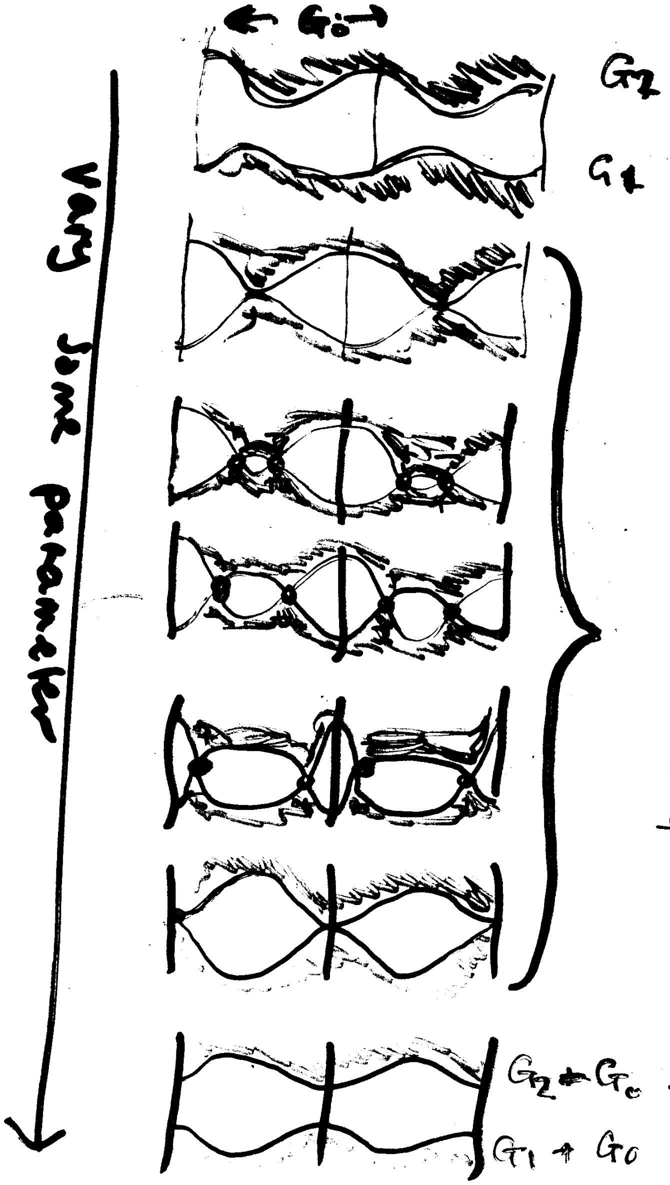
$\mathbb{C}_1' = \mathbb{C}_1 - n$

$\mathbb{C}_1' + \mathbb{C}_2' = \mathbb{C}_1 + \mathbb{C}_2$

Vary 3 parameters to get a degeneracy of a complex Hermitian matrix

$(k_x \,;\, k_y \,;\, g)$

Single value g_c of g at which bands are degenerate



FINITE RANGE of g where BANDS CONNECTED BY DIRAC POINTS (±)

G_1, G_2 not defined, but $G_1 + G_2$ is.

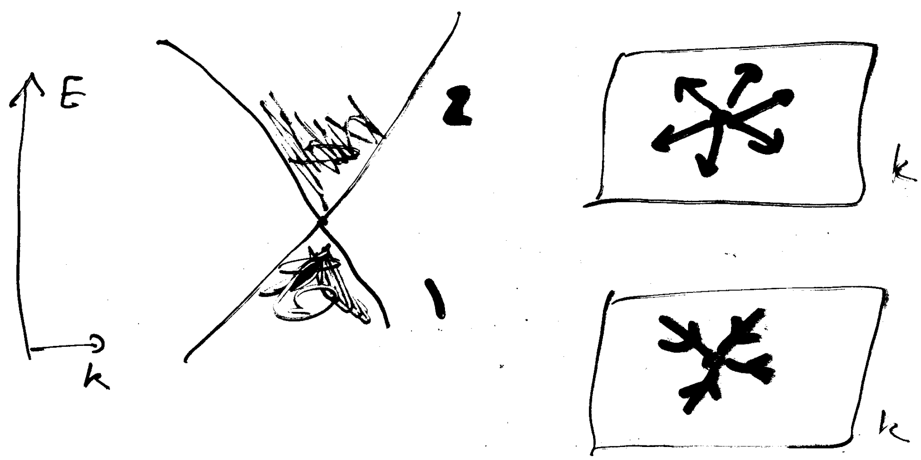
Vary (k_x, k_y, k_z) to find degeneracy points

$$\vec{G}_1 + \vec{G}_2 = \vec{G}_1' + \vec{G}_2'$$

3D Dirac point is Chiral

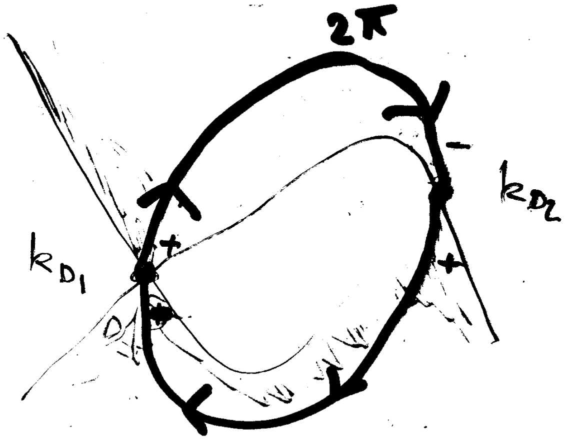
$$\underline{\underline{H}}^{eff} = \sum_{i=1}^{3} A^i(\underline{k})\, \underline{\underline{\sigma}}^i_{pauli} \qquad A^i(k) \text{ vanishes linearly at } k_D$$

$$\mathrm{sgn}\left(\det \left.\frac{\partial A^i}{\partial k_j}\right|_{k_D}\right) = \pm 1$$



- monopole source $\pm 2\pi$ of Berry curvature at $\vec{k}_{D\pm}$ in band 1
- monopole source $\mp 2\pi$ in band 2 at same $k_{D\mp}$

• 2 Dirac points of opposite chirality. k_{D+}, k_{D-}



Degenerate 3D band are
Connected by a 2π Berry Curvature
"Flux loop".

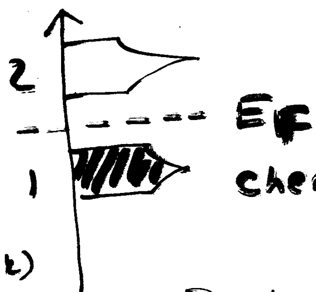
$\approx$ "WORMHOLES" BETWEEN UNIVERSES,
with a flux quantum passing
Through

2D Quantum Hall Effect

(Integer QHE with $\vec{B}=0$, but
Broken time-reversal symmetry)

FDMH (1988)

$$\sigma^{xy} = \frac{e^2}{2\pi\hbar}\,\nu$$



chern number C_1

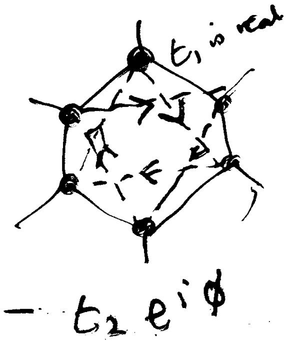
$$\nu = \int_{BZ} d^2k \sum_n F_n^{xy}(k)\, n_n(k)$$

occupation number

Bulk medium has gap at Fermi energy (gapless EDGE STATES at E_F exist)

$$\nu = \sum_{\text{occupied bands}} C_n = \text{integer}$$

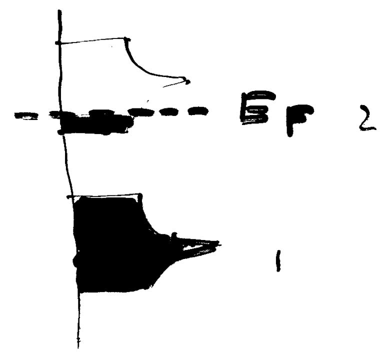
Chiral



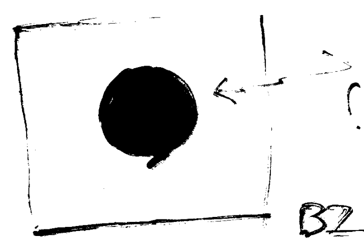
2D "graphene" with complex 2nd neighbor hopping, real 1st neighbor hopping

$- - \rightarrow - \; t_2 e^{i\phi}$

2D Anomalous Hall effect (metal)



$$\nu = \frac{1}{2\pi}\int_{BZ} d^2k \; F_1^{xy}(k) + \frac{1}{2\pi}\int_{FS} d^2k \; F_2^{xy}(k)$$



$$\frac{1}{2\pi}\int_{FS} d^2k \; F_2^{xy} = \frac{1}{2\pi}\oint \nabla^x A_2^y - \nabla^y A_2^x = \frac{\Phi^F_{Berry}}{2\pi}(FS\,orbit)$$

$$\nu = \mathbb{C}_1 + \frac{\Phi_2^F}{2\pi}$$

NON QUANTIZED (NON-INTEGER) PART OF ν IS COMPLETELY DETERMINED AT FERMI LEVEL

3D case

$$\sigma_D^{ab} = \frac{e^2}{(2\pi)^2 \hbar} \epsilon^{abc} K_c$$

(Integer) QHE $\vec{K} = \vec{G}$ (reciprocal vector)

anomalous (metallic) QHE:

non quantized part $\vec{K} \bmod \vec{G}$ is completely determined at Fermi Surface

---

electron density in insulator is $\frac{n}{\Omega}$ $\leftarrow$ integer; $\Omega \leftarrow$ volume of unit cell

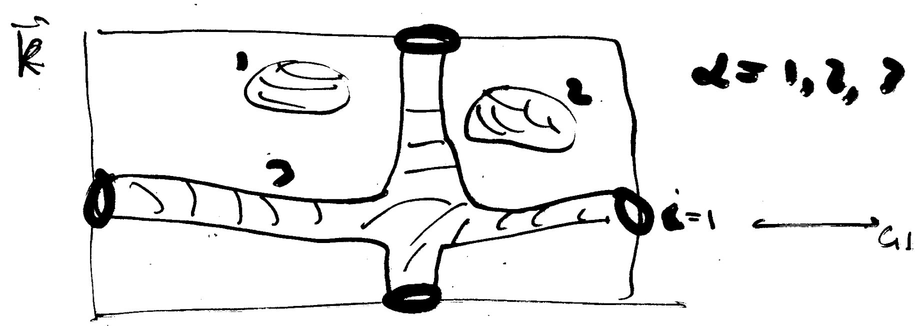
in metal

electron density (modulo $\frac{1}{\Omega}$)

– is determined by the volume of the Fermi Surface

("non quantized part")

- Fermi surface may be split up into independent manifolds



$\alpha = 1, 2, 3$

$$\vec{K} = \sum_\alpha \vec{K}_\alpha$$

density $$\rho = \sum_\alpha \rho_\alpha$$

locally adiabatically conserved density if $\mathbb{C}_\alpha$ (Chern number) $= 0$!

- $$\vec{K}_\alpha = \frac{1}{2\pi}\int_{S_\alpha} ds^\mu \wedge ds^\nu \, F_{\mu\nu}(\underline{s}) \, \vec{k}_{F\alpha}(s) + \sum_i \frac{\phi_{i\alpha}}{2\pi} \vec{G}_{i\alpha}$$

- $$\frac{1}{2\pi}\int_{S_\alpha} ds^\mu \wedge ds^\nu \, F_{\mu\nu}(s) = \mathbb{C}_\alpha$$

Each Fermi surface piece is a compact 2D manifold

→ HAS A CHERN NUMBER!

What about Fermi surfaces with non-zero chern number?

① expression must be gauge invariant

gauge (electromagnetic gauge) transformation

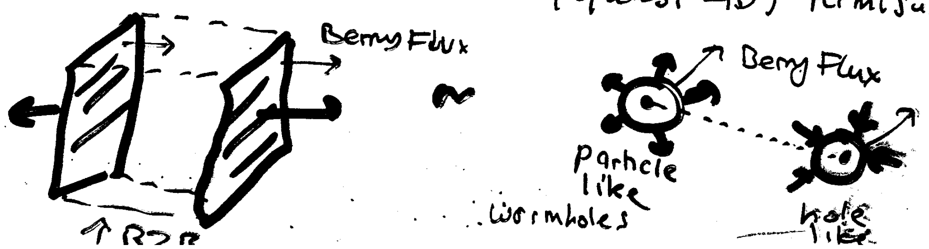
$$\vec{k}_{F\alpha}(\vec{s},r) \rightarrow \vec{k}_{F\alpha}(\vec{s},r) - \frac{e}{\hbar}\vec{A}(r)$$

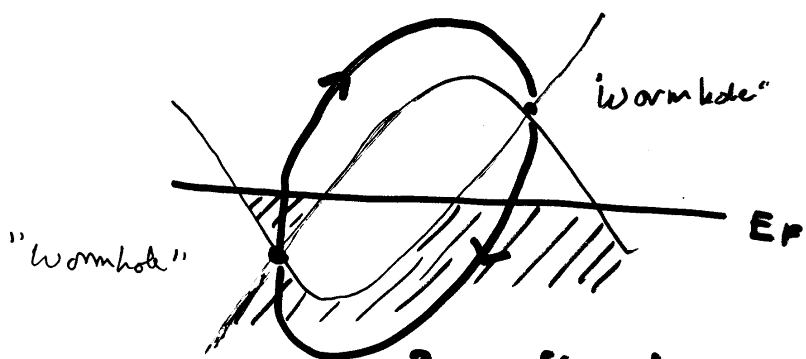
$$\vec{K} = \frac{1}{2\pi}\int_{S^1} ds^\mu \wedge ds^\nu\, F_{\mu\nu}(\omega)\, \vec{k}_F + \sum \frac{\phi}{2\pi}\vec{G}$$

$$\longrightarrow \vec{K} + \left(\sum_\alpha \mathbb{C}_\alpha\right) e/\hbar\, \vec{A}(r)$$

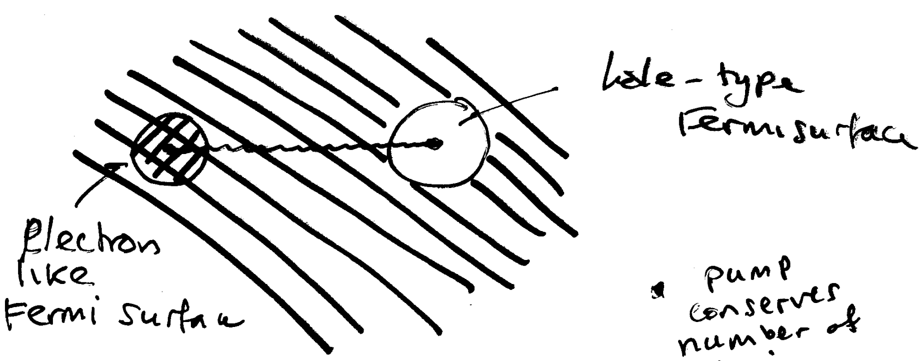
- must have $\sum_\alpha C_\alpha = 0$
- but suppose we have $\mathbb{C}_1 + \mathbb{C}_2 = 0$, $\mathbb{C}_1 = -\mathbb{C}_2 \neq 0$?

$\longrightarrow$ WORMHOLES!
or Chiral (quasi 1D) Fermi Surface

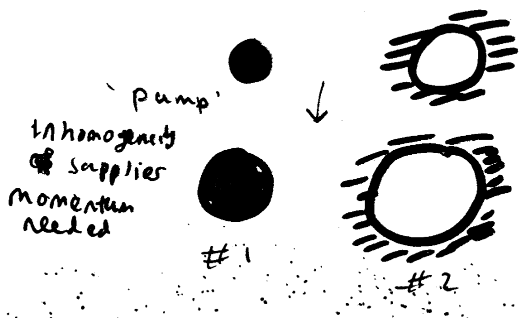




Berry flux loop (flux 2π)



• pump conserves number of states in each band



equal numbers of particles added to Fermi sea #1 and holes added to #2

NO NET Charge added

Streda Formula

$$\left.\frac{\partial \rho_e}{\partial \vec{B}}\right)_\mu = \frac{e^2}{(2\pi)^2\hbar} \vec{K}(\mu)$$

- add a uniform magnetic field. at Fixed chemical potential μ

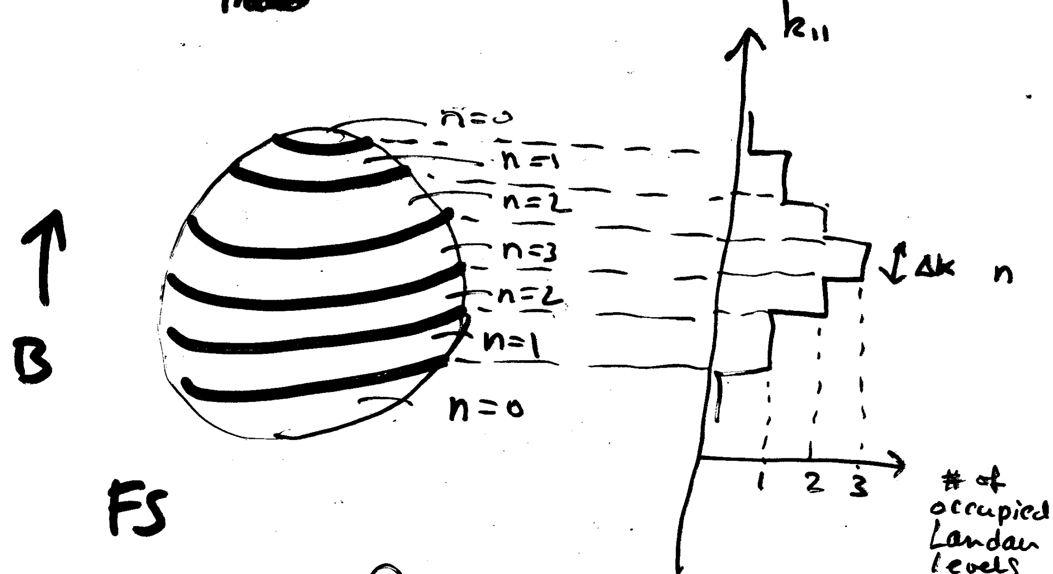
  $\vec{K}(\mu)$ measures linear response of electric Charge density.

- easily shown from Semiclassical quantization in presence of Berry Phase

$$\underbrace{A(k_{\parallel})}_{\substack{\text{Fermi surface}\\ \text{Cross section}\\ \perp \text{ to } \vec{B}}} \ell^2 - \underbrace{\phi(k_{\parallel})}_{\substack{\text{Berry}\\ \text{Phase}\\ \text{of FS}\\ \text{orbit}}} = 2\pi(\underbrace{n}_{\text{integer}}+\tfrac{1}{2})$$

$\ell^2 = \frac{\hbar}{eB}$

metal



$$\rho = e \frac{1}{2\pi\ell^2} \sum_i n_i \Delta k_i$$

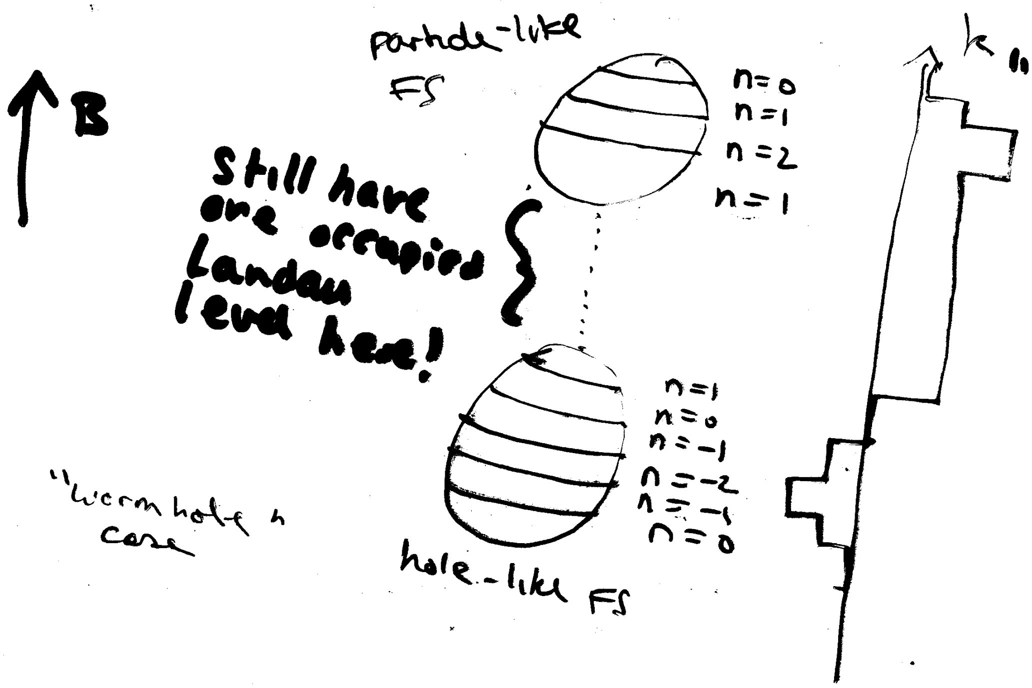
One-D Fermi gases moving along magnetic field lines

(a) switch on electron electron interactions

- relation between k_F and electron density doesn't change (Luttinger Theorem)
- $\vec{k}$ is robust against quasiparticle interactions!
- A true Fermi liquid property

Interacting electron occupations

Semiclassical quantization with non-zero Chern number



"wormhole" case

- MORE STUFF

--- "Spin-Hall effect" (proposed spin analog of AHE)

- Středa says "No" it doesnt exist if Time-reversal sym. is unbroken.

$$\left.\frac{\partial S^i}{\partial B^a}\right)_\mu = \frac{e}{(2\pi)^2} \cdot K^i_a(\mu)$$

$$J^{ia} = \epsilon^{abc} K^i_c E_b$$

- but $K^z_a(\mu) = 0$ in Rashba S.O.C. model...

($S^i \propto B^3$ not B!)
Spin density

AHE WORK available at
Cond-mat/0408417