Berry's Phase and the Quantum Geometry of the Fermi Surface

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See: F. D. M. Haldane, Phys. Rev. Lett. **93**, 206602 (2004) (cond-mat/0408417)

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v 1.0

What is the Fermi surface of metals?

- "A surface in k-space separating empty and filled states at T=0" (free electron viewpoint)

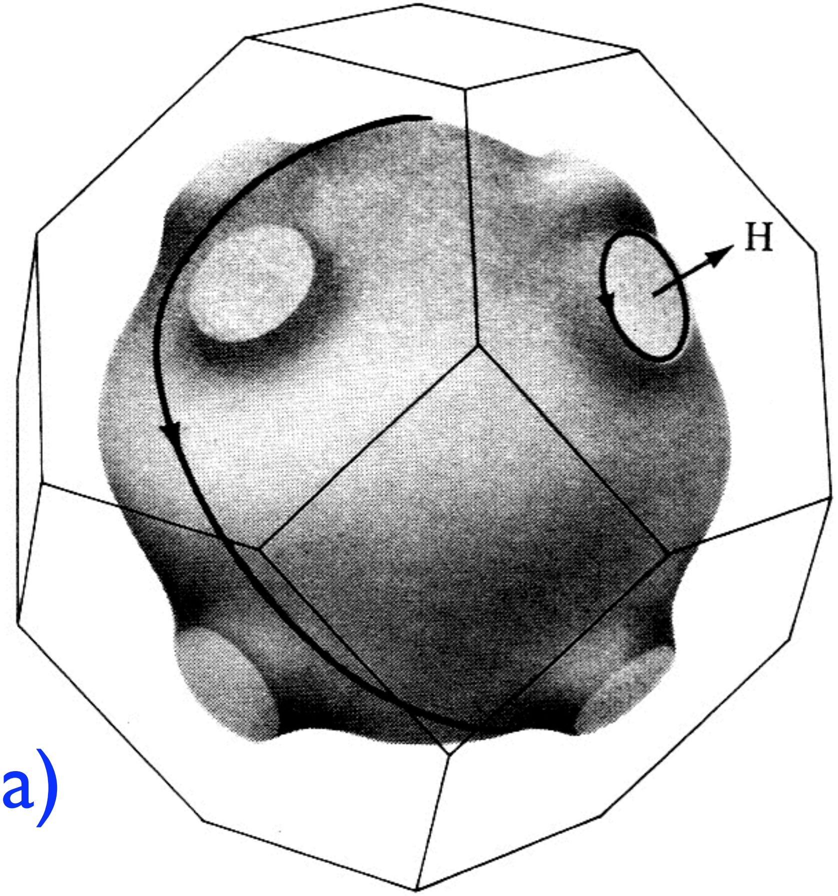
or

- "A set of one or more compact 2-dimensional manifolds on which long-lived quasiparticle states can flow in response to applied fields" (a "quantum geometric" viewpoint.)

I will describe the second "intrinsic" geometric viewpoint where previously unnoticed aspects of the Fermi surface "emerge".

leads to the solution of a 110 year-old puzzle: the origin of the "Anomalous Hall effect" in ferromagnetic metals , now seen to be a quasiparticle Berry phase effect!

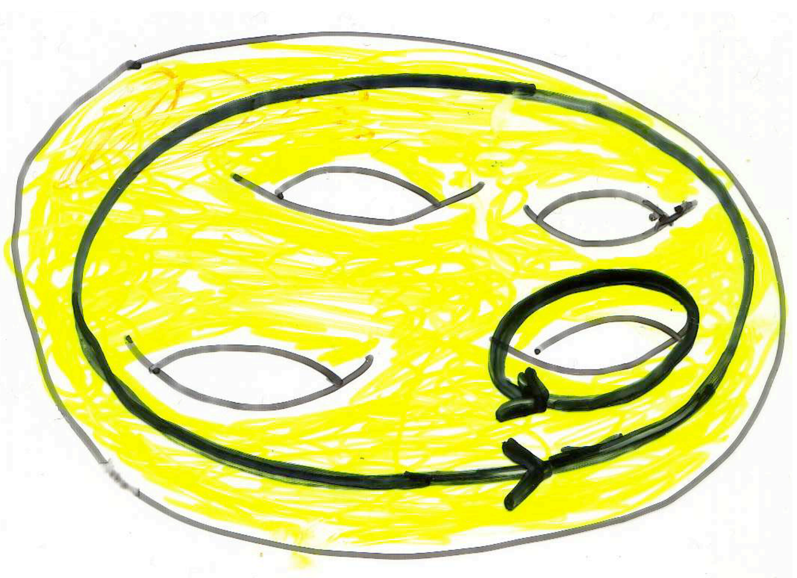
Fermi surface of a noble metal (silver):



(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

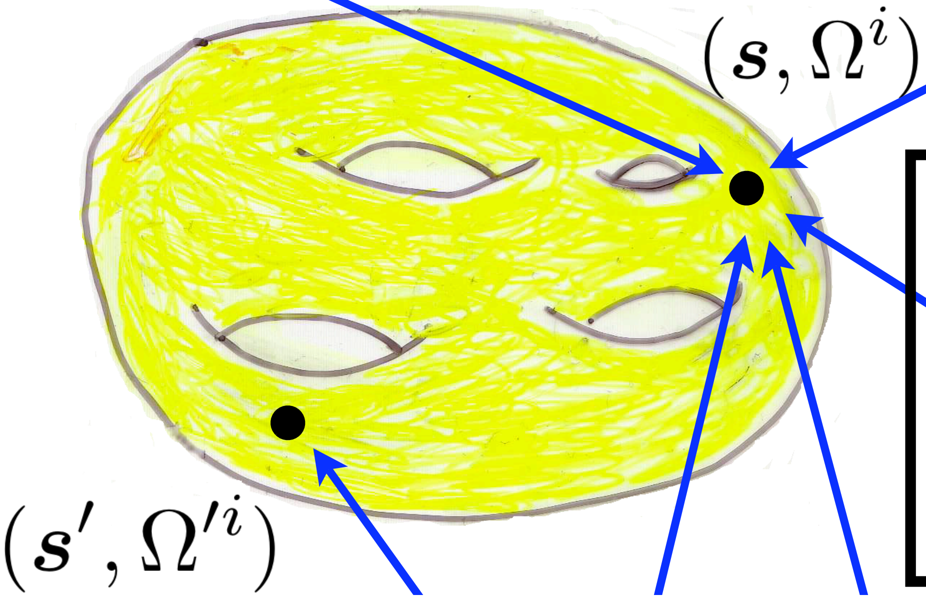
k-space metric

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

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:

$\left\{ \begin{array}{ll} \text{Z(2) + SO(3)} & g_s = 2 \\ \text{U(1)} & g_s = 1 \end{array} \right.$

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”

$$\mathcal{G}^{H}_{\mu\nu}(\boldsymbol{s})$$

$$\mathcal{A}_{\mu}(\boldsymbol{s})\,\mathcal{A}^{i}_{\mu}(\boldsymbol{s})$$

Hilbert-space metric

Berry gauge fields:

$\left\{\begin{array}{l}\text{Z(2) + SO(3)} \quad g_s = 2 \\ \text{U(1)} \quad g_s = 1\end{array}\right.$

if both spatial inversion and time-reversal symmetry are present* → $g_s = 2$

otherwise* → $g_s = 1$

* assumes spin-orbit coupling

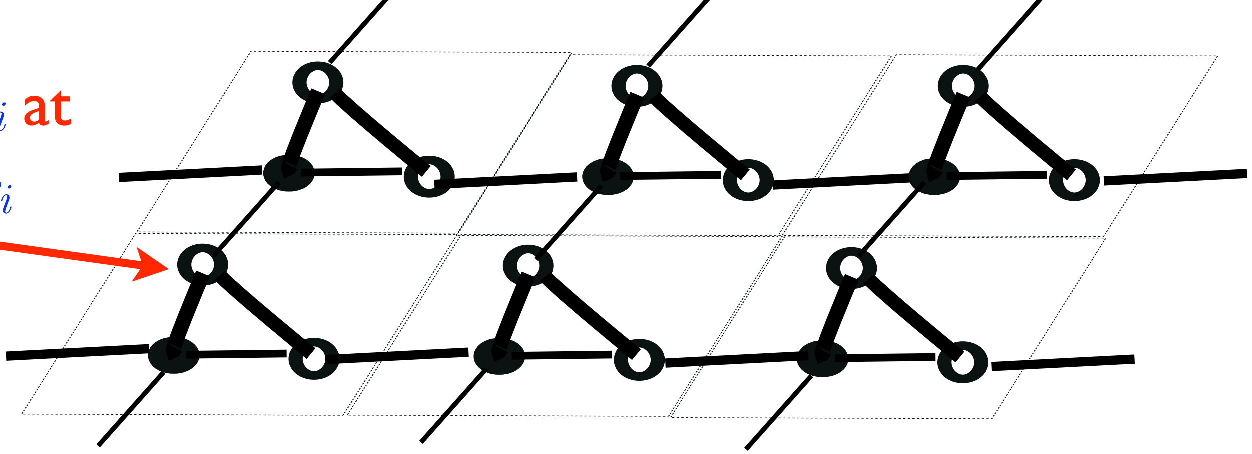
- The Hilbert-space metric and the Berry gauge fields modify the ballistic behavior of quasiparticles which are accelerated by quasi-uniform electromagnetic fields, chemical potential and thermal gradients, strain fields, etc.

- Hilbert space geometric effects are completely omitted in a single-band approximation that also neglects spin-orbit coupling (like a one-band Hubbard model).

New Physics that emerges:

found so far:

- (Intrinsic) Anomalous Hall Effect in Ferromagnetic metals: the recently-validated Karplus-Luttinger (1954) theory is now seen as a Fermi surface geometry effect! (FDMH, Phys. Rev. Lett. 93, 206602 (2004))
- "Composite Fermion" Fermi liquids at ν = 1/2m lowest Landau level filling also exhibit an AHE.



Orbital $c^{\dagger}{}_i$ at position $\boldsymbol{r}_i$

network of electronic orbitals tied to positions of atomic nuclei

- for new effects, need at least TWO orbitals in the unit cell.

- Specify (a) Hamiltonian matrix elements on network AND (b) embedding of orbitals in real space continuum (needed for coupling to slowly-varying electromagnetic fields, thermal gradients, etc.)

(a)
$$H_0(\{h_{ij}\}) = \sum_{ij} h_{ij} c_i^{\dagger} c_j$$

$$H = H_0 + H_{\mathrm{int}}$$
$$[H_{\mathrm{int}}, U(\boldsymbol{k})] = 0$$

(b)
$$U(\boldsymbol{k};\{\boldsymbol{r}_i\}) = \prod_i \left(c_i c_i^{\dagger} + e^{i\boldsymbol{k}\cdot\boldsymbol{r}_i} c_i^{\dagger} c_i \right)$$

gauge-invariant interactions (origin of frequency-dependent self-energy)

Matsubara single-electron (finite-temperature) Green's function:

(0 < τ < β is "imaginary time")

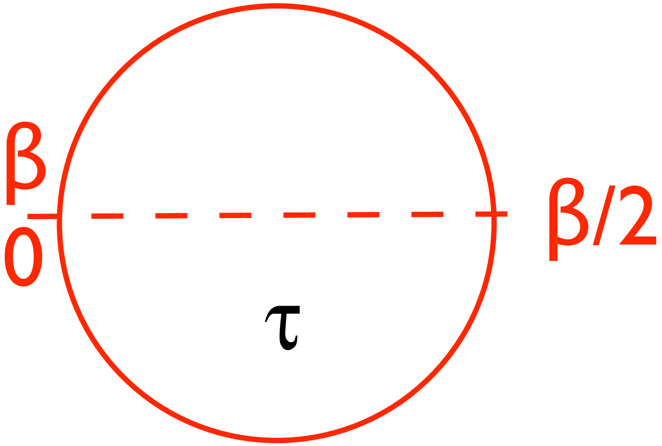
$$\mathcal{G}_{ij}(\tau) = -\langle T_\tau c_i(\tau) c_j^\dagger \rangle_{\beta\mathcal{H}} \longleftarrow \mathcal{H} = H - \mu N$$

$c^\dagger{}_i$ creates an electron in an orbital that is physically located at a real-space position $\boldsymbol{r}_i$

When τ = β/2 (the largest imaginary-time separation), the Green's function is Hermitian !

$$\mathcal{G}_{ij}(\tfrac{1}{2}\beta) = \mathcal{G}^*_{ji}(\tfrac{1}{2}\beta)$$

$$\mathcal{G}_{ij}(\beta/2) = \frac{\mathrm{Tr}\left(e^{-\beta\mathcal{H}/2} c_i e^{-\beta\mathcal{H}/2} c_j^\dagger\right)}{\mathrm{Tr}\, e^{-\beta\mathcal{H}}}$$



- <u>Fundamental eigenproblem that will define the Fermi surface:</u>

Equilibrium property of an interacting many-particle system.

$$\boxed{\mathcal{G}_{ij}(\tfrac{1}{2}\beta)\Psi_{\nu j} = \mathcal{G}_{\nu}\Psi_{\nu i}}$$

in one-particle Hilbert space

$$\mathcal{G}_{ij}(\tfrac{1}{2}\beta) = \mathcal{G}^{*}_{ji}(\tfrac{1}{2}\beta)$$

real eigenvalues

orthogonal eigenstates

Bloch character of eigenstates:

- $\mathcal{G}_{ij}$ depends only on $\mathcal{H}$, but indices i,j range over all orbitals; replace by:

$$\mathcal{G}_{ij}(\boldsymbol{k};\tfrac{1}{2}\beta) \equiv \mathcal{G}_{ij}(\tfrac{1}{2}\beta)e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_j-\boldsymbol{r}_i)}$$

- This now also depends on the real-space positions $\boldsymbol{r}_i$ of the orbitals, but now indices i,j just range over orbitals in the unit cell (includes spin)

$$\boxed{\mathcal{G}_{ij}(\boldsymbol{k};\tfrac{1}{2}\beta)u(\boldsymbol{k})_{\nu j} = \mathcal{G}_{\nu}(\boldsymbol{k})u(\boldsymbol{k})_{\nu i}}$$

$$\Psi(\boldsymbol{k})_{\nu i} = e^{i\boldsymbol{k}\cdot\boldsymbol{r}_i}u(\boldsymbol{k})_{\nu i} \longleftarrow \text{Full Bloch state}$$

(property of Hamiltonian alone)

(embedding-dependent factorization)

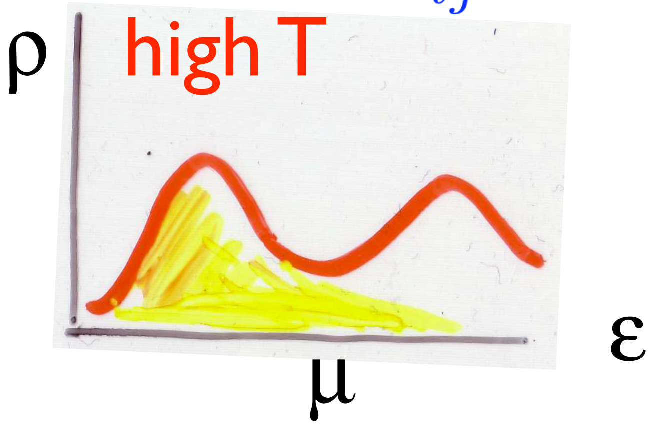
Lehmann representation

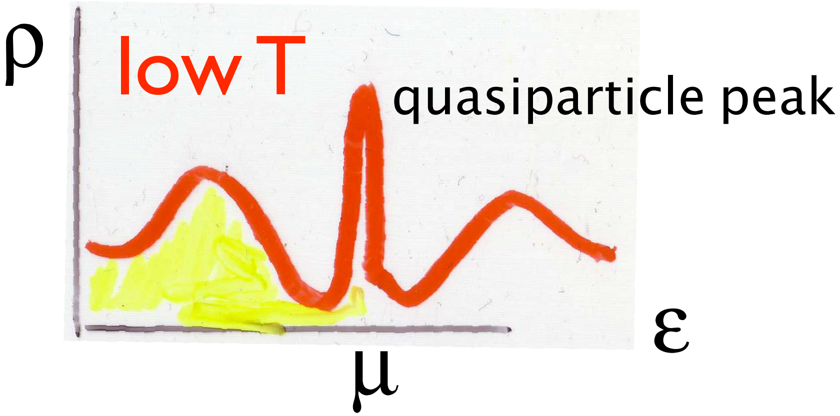
$$\mathcal{G}_{ij}(\boldsymbol{k},\tfrac{1}{2}\beta) = \int_{-\infty}^{\infty} A_{ij}(\varepsilon,\boldsymbol{k};T)\left(\tfrac{1}{2}\beta\,\mathrm{sech}\,\tfrac{1}{2}\beta(\varepsilon-\mu)\right)$$

concentrated near ε =μ at low T!

- For interacting electrons, at finite T, $A_{ij}(\varepsilon,\ k\ ;T)$ is a positive-definite Hermitian matrix, but cannot be simultaneously diagonalized at different ε
- Gauge-invariant local density of states (seen in photoemission/absorbtion):

$$\rho(\varepsilon,\boldsymbol{r},T) = \sum_{ij} \delta_{\boldsymbol{r},\boldsymbol{r}_i}\delta_{\boldsymbol{r},\boldsymbol{r}_j} \int_{\mathrm{BZ}} \frac{d^3\boldsymbol{k}}{(2\pi)^3} A_{ij}(\varepsilon,\boldsymbol{k};T)$$





$$\mathcal{G}_{ij}(\boldsymbol{k},\tfrac{1}{2}\beta) = \int_{-\infty}^{\infty} A_{ij}(\varepsilon,\boldsymbol{k};T)\left(\tfrac{1}{2}\beta\,\mathrm{sech}\,\tfrac{1}{2}\beta(\varepsilon-\mu)\right)$$

concentrated
near ε =μ
at low T!

- For non-interacting electrons, diagonalizing $\mathcal{G}_{ij}\,(\boldsymbol{k},\,½\beta)$ is equivalent to diagonalizing the one-body Hamiltonian:

$$h_{ij}(\boldsymbol{k})u_{nj}(\boldsymbol{k}) = \varepsilon_n(\boldsymbol{k})u_{ni}(\boldsymbol{k}) \qquad h_{ij}(\boldsymbol{k}) \equiv h_{ij}e^{i\boldsymbol{k}\cdot(\boldsymbol{r}_j-\boldsymbol{r}_i)}$$

$$\mathcal{G}_{ij}(\boldsymbol{k};\tfrac{1}{2}\beta)u_{nj}(\boldsymbol{k}) = \mathcal{G}_n(\boldsymbol{k})u_{ni}(\boldsymbol{k})$$

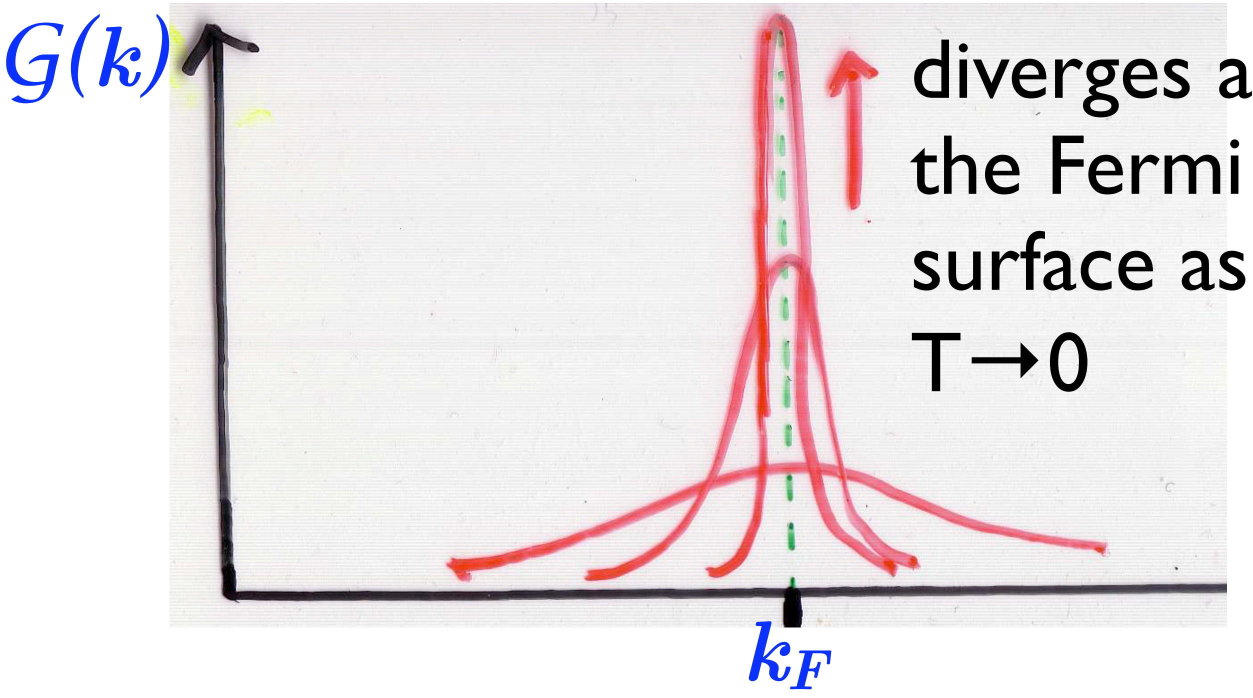
$$\boxed{\mathcal{G}_n(\boldsymbol{k}) = \tfrac{1}{2}\beta\,\mathrm{sech}\,\tfrac{1}{2}\beta(\varepsilon_n(\boldsymbol{k})-\mu)}$$

as T→0, this diverges if **k** is on the Fermi surface, but vanishes otherwise.

eigenvalue of the non-interacting system Green’s function

Divergence of the eigenvalue of the Green's function signals the formation and location of the Fermi surface

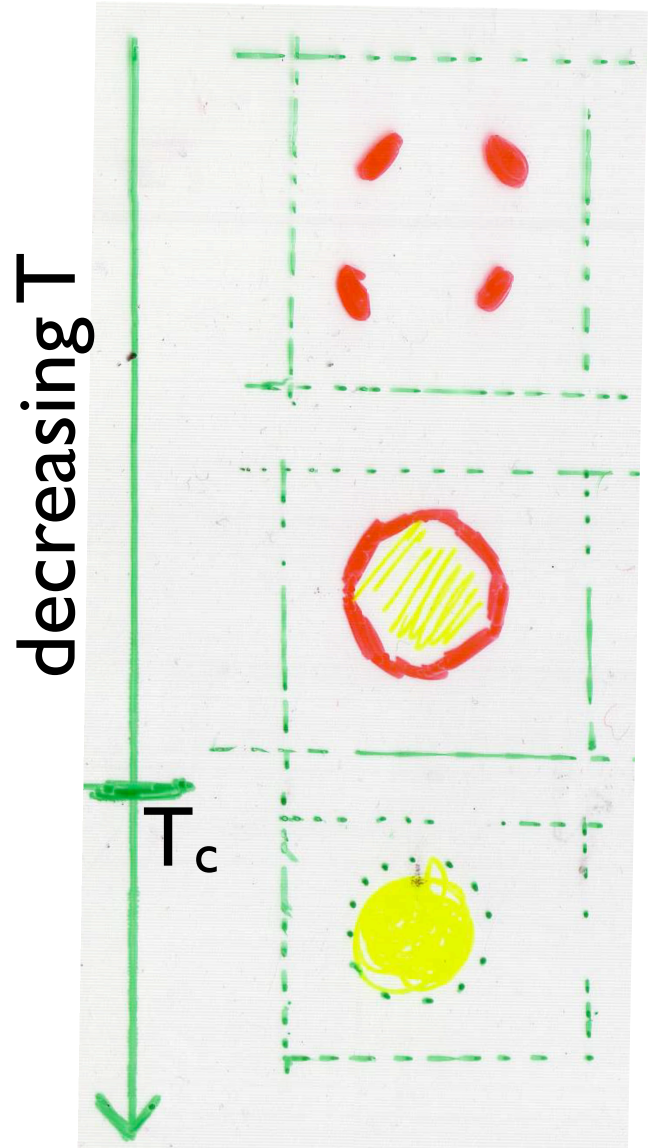
$$\mathcal{G}_n(\boldsymbol{k}) = \tfrac{1}{2}\beta\,\mathrm{sech}\,\tfrac{1}{2}\beta(\varepsilon_n(\boldsymbol{k}) - \mu)$$



diverges at the Fermi surface as T→0

In Fermi liquid theory, the eigenvalue becomes large at low T for k near k_F, but eventually decreases again when the BCS transition to superconductivity occurs...

Scenario for a normal metal as it is cooled:



(a) "cold spots" with a large eigenvalue of $\mathcal{G}_{ij}(\frac{1}{2}\beta)$ (and a quasiparticle with a inelastic mean free path much longer than unit-cell dimensions) form in isolated regions of the Brillouin zone.

(b) The "cold spots" link up to form a connected region of long-lived quasiparticles. Their mean free path is long enough for the surface to be measurable with the De Haas-Van Alpen effect. This is a degenerate Fermi liquid.

(c) The BCS transition to weak-coupling superconductivity destroys the Fermi surface by opening a gap.

In high-T_c materials, the transition to strong-coupling superconductivity may occur at stage (a) (are these "cold spots" the "Fermi arcs"?)

k-space Fermi-surface geometry:

- **s** = (s^1,s^2) is a 2-component curvilinear parameterization of the Fermi surface.
- **k**$_F$(**s**) is a "dangerous variable", only defined modulo a reciprocal vector **G**, and is not gauge invariant:

$$e^{i(\boldsymbol{k}_F(\boldsymbol{s})-\boldsymbol{k}_F(\boldsymbol{s}'))\cdot\boldsymbol{R}} \longleftarrow$$

Only this combination is physically-meaningful: (**R** is any periodic lattice translation)

- **n**$_F$(**s**) is the (unit vector) direction of motion of the quasiparticle in real space, if **s** is not changing with time.

Hilbert space geometry

- There is a natural definition of "distance" in Hilbert space:

$$D(|\Psi_1\rangle, |\Psi_2\rangle)^2 = 1 - |\langle\Psi_1|\Psi_2\rangle|$$

- "Pure-state" limit Bures-Uhlmann distance between density matrices. max D = 1 (orthogonal states)
- satisfies symmetry, triangle inequality.
- Berry gauge invariant: D_{12} = 0 iff states are physically equivalent:

(U(1) gauge equivalence)

$$D_{12} = 0 \rightarrow |\Psi_2\rangle = e^{i\chi}|\Psi_1\rangle$$

Manifold of quantum states

- Let **g** = (g^1,g^2,....,g^d) (real) parameterize a d-dimensional manifold, and $|\Psi(\mathbf{g})\rangle$ be a state in a D-dimensional Hilbert space with d ≤2(N-1)
- The covariant derivative is:

$$
\begin{aligned}
|\Psi(\boldsymbol{g})\rangle &= \sum_i u_i(\boldsymbol{g})|i\rangle, \quad \langle i|j\rangle = \delta_{ij} \\
|\partial_\mu \Psi(\boldsymbol{g})\rangle &= \sum_i \partial_\mu u_i(\boldsymbol{g})|i\rangle, \quad \partial_\mu \equiv \frac{\partial}{\partial g^\mu} \\
\mathcal{A}_\mu(\boldsymbol{g}) &= -i\langle\Psi|\partial_\mu\Psi\rangle \longleftarrow \text{U(1) Berry connection} \\
|D_\mu \Psi(\boldsymbol{g})\rangle &= |\partial_\mu \Psi\rangle - i\mathcal{A}_\mu|\Psi\rangle, \quad \langle\Psi|D_\mu\Psi\rangle = 0.
\end{aligned}
$$

Berry connection is a “vector potential” in g-space!

Riemannian metric structure (Provost and Vallee 1980)

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

- Positive Hermitian matrix (definite provided $\mathcal{G}_{\mu\nu}$ is non-singular, generic case)
- $\mathcal{G}_{\mu\nu}$ is a real symmetric metric tensor, derives from the Bures-Uhlmann distance.
- $\mathcal{G}^{\mu\sigma}\mathcal{G}_{\sigma\nu} = \delta^\mu_\nu$
- $\mathcal{F}_{\mu\nu} = \partial_\mu \mathcal{A}_\nu - \partial_\nu \mathcal{A}_\mu$ is the Berry Curvature

(analog of magnetic flux density in g-space!)

$$\mathcal{G}_{\mu\nu} \geq \mathcal{G}^{\sigma\tau}\mathcal{F}_{\mu\sigma}\mathcal{F}_{\nu\tau}$$

analog of electromagnetic stress-energy tensor?

$$\boxed{\mathcal{F}_{\mu\nu}(\boldsymbol{g}) = \mathcal{F}(\boldsymbol{g})|\det \mathcal{G}|^{1/2}\epsilon_{\mu\nu} \quad |\mathcal{F}(\boldsymbol{s})|^2 \leq 1}$$

special form for a 2-manifold

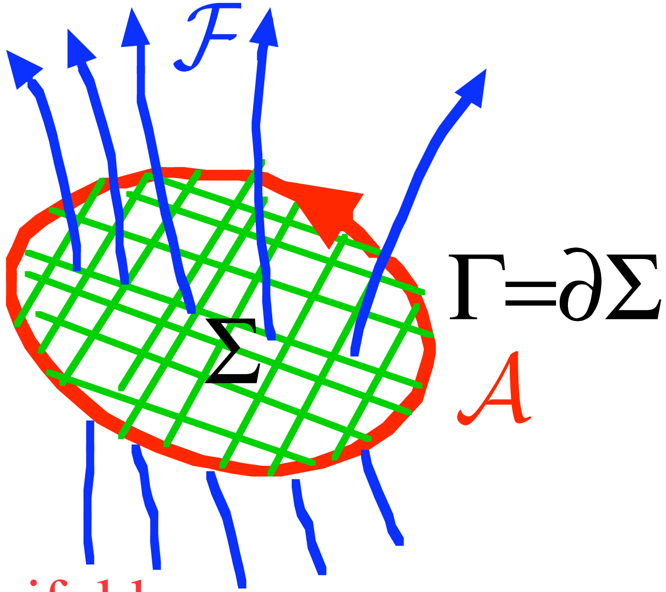
Berry curvature

- (Berry 1984, Simon 1983, TKNN 1982) ; now much more familiar than the Riemannian metric structure.
  - Berry curvature is analog of magnetic flux density (satisfies Gauss law)
  - Berry connection is analog of magnetic vector potential
  - First Chern invariant is analog of Dirac magnetic monopole quantization.....

U(1) **Berry "gauge field" on the manifold**

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

$$= \exp i \int_\Sigma \mathcal{F}_{\mu\nu}(\boldsymbol{g}) dg^\mu \wedge dg^\nu$$

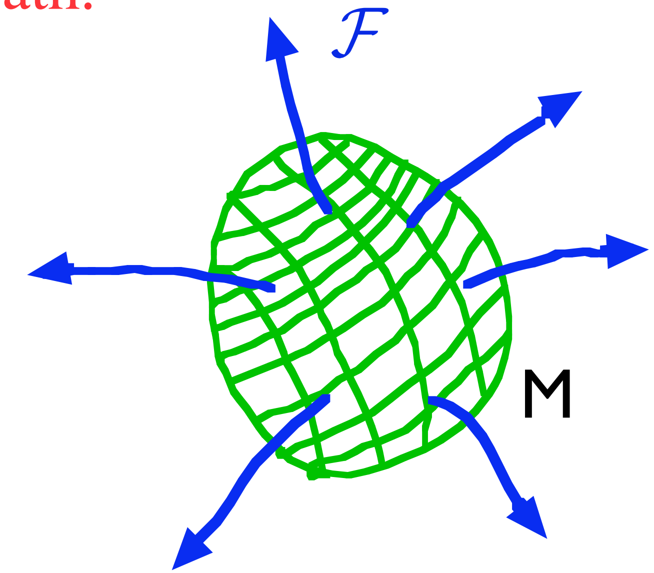


Berry 1984

Berry's phase for a closed directed path on the manifold can be obtained from the integral of the Berry curvature over any oriented 2-manifold bounded by the path.

$$\frac{1}{2\pi} \oint_M \mathcal{F}_{\mu\nu}(\boldsymbol{g}) dg^\mu \wedge dg^\nu = C^{(1)}(M)$$

The integral of Berry curvature over a ***closed*** 2-submanifold M gives the ***integer*** "***Chern number***" topological invariant of M ("first Chern class"),



Application to the Fermi surface

- “old” (k-space) geometry” $\mathbf{k}_F(\mathbf{s})$, $\mathbf{n}_F(\mathbf{s})$.
- “new” (Hilbert space) geometry: $\mathcal{G}_{\mu\nu}(\mathbf{s})$, (Riemann metric), plus $\mathcal{A}_\mu(\mathbf{s})$ (U(1) Abelian “gauge potential”)
- if the Fermi surface is spin-split: this U(1) gauge potential becomes a topological Z(2) “gauge potential” if the Fermi surface is not spin split (both spatial inversion and time-reversal unbroken), but an additional SO(3) non-Abelian gauge potential $\mathcal{A}^i{}_\mu(\mathbf{s})$ appears if spin-orbit coupling is present.

relation to embedding in space

- On the Fermi surface, the metric $\mathcal{G}_{\mu\nu}(\mathbf{s})$, and Berry connection(s) $\mathcal{A}_{\mu}(\mathbf{s})$ ($\mathcal{A}^{i}{}_{\mu}(\mathbf{s})$) are not quite the "standard" ones, because they characterize the geometry of its embedding of the electronic system in continuum space, as well as its Hamiltonian.
- (only the Topological invariants are independent of the embedding)

Hall effect in 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$_2$Se$_{4-x}$Br$_x$.

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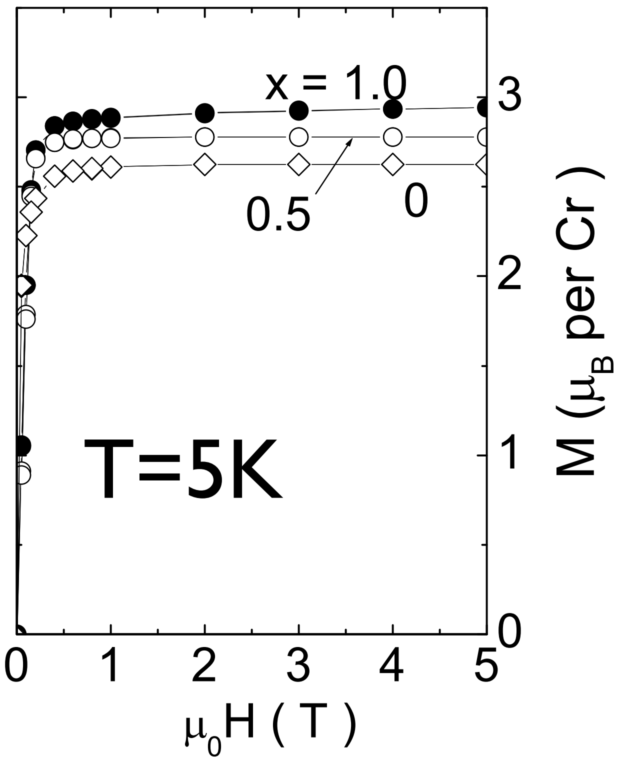
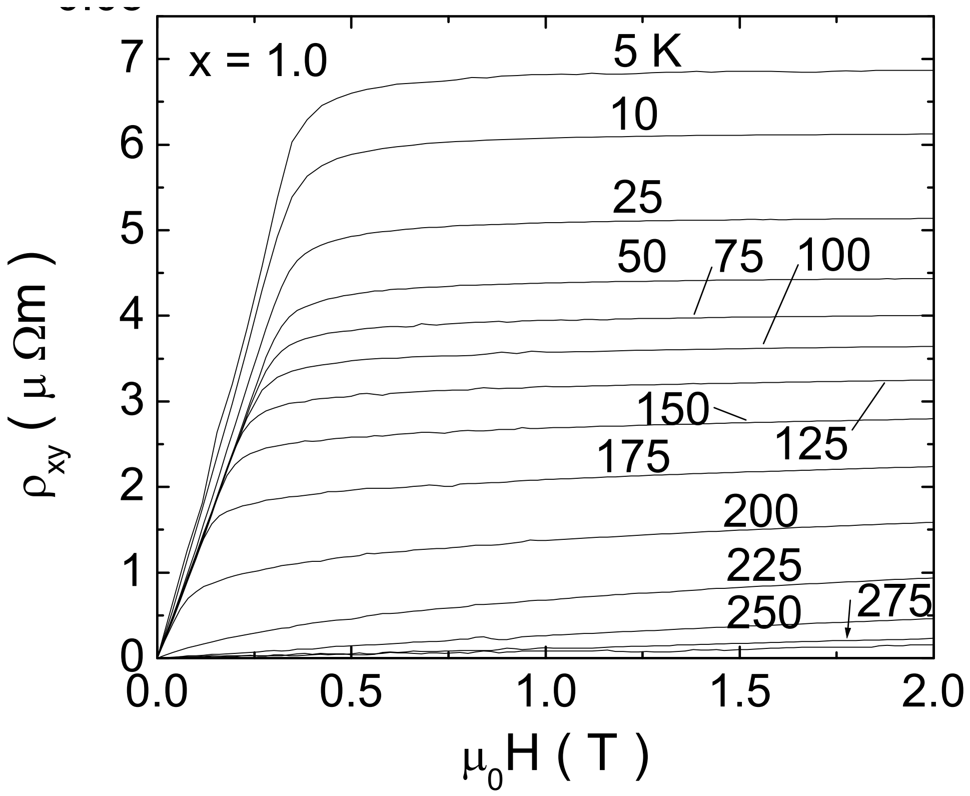




example of a very large AHE

- 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.)

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 →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!

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.)

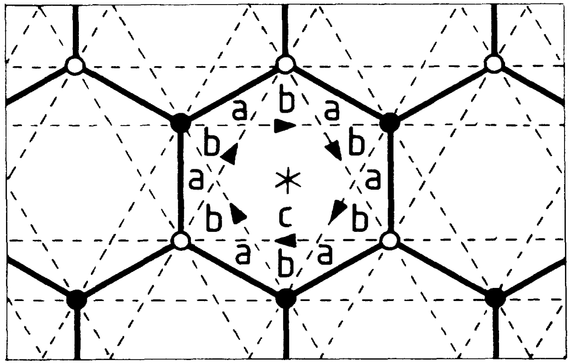


FIG. 1. The honeycomb-net model ("2D graphite") showing nearest-neighbor bonds (solid lines) and second-neighbor bonds (dashed lines). Open and solid points, respectively, mark the A and B sublattice sites. The Wigner-Seitz unit cell is conveniently centered on the point of sixfold rotation symmetry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

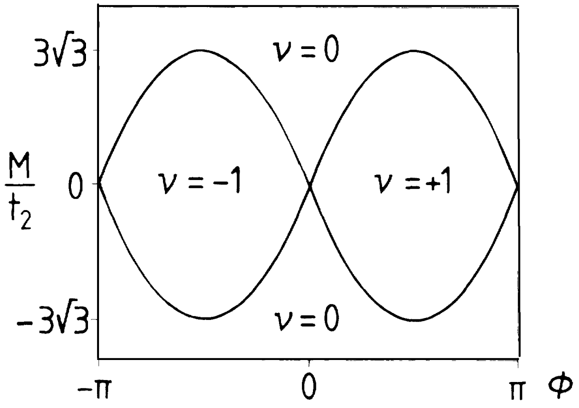


FIG. 2. Phase diagram of the spinless electron model with $|t_2/t_1| < \frac{1}{3}$. Zero-field quantum Hall effect phases ($\nu = \pm 1$, where $\sigma^{xy} = \nu e^2/h$) occur if $|M/t_2| < 3\sqrt{3}|\sin\phi|$. This figure assumes that t_2 is positive; if it is negative, ν changes sign. At the phase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

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

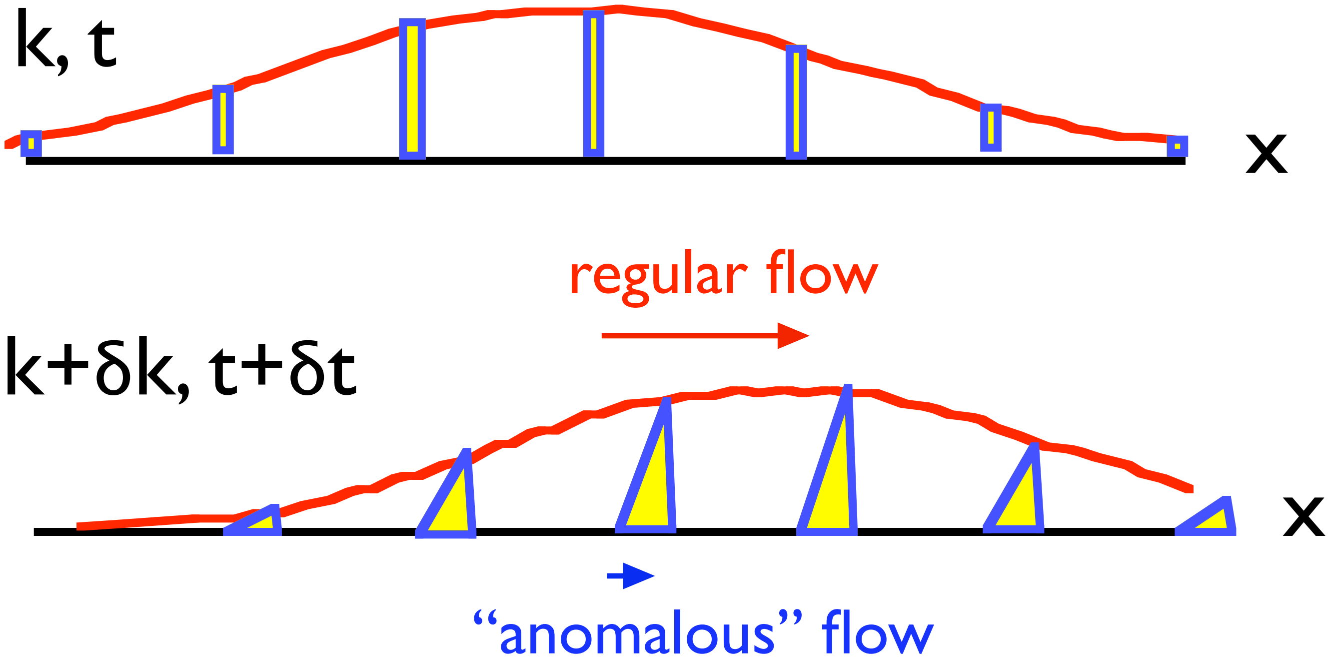
$$F_{ab}(\boldsymbol{r}) = \epsilon_{abc}B^c(\boldsymbol{r})$$

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 ($a \in \{x,y,z\}$).

Current flow as a Bloch wavepacket is accelerated



- If the Bloch vector ***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 ***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 ***k*** changes, and ***the anomalous velocity term vanishes***.

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!)

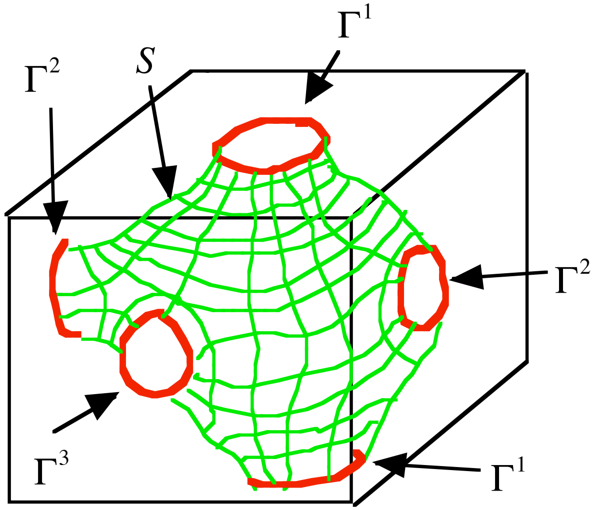
non-quantized part of 3D case can also be expressed as a Fermi surface integral

- **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

- 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 ω→0, T→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 QED3 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 corrections to the 2D QHE.

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

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.
- After 43 years, the famous Luttinger (1961) theorem relating the non-quantized part of the electron density to the Fermi surface volume now has a “partner”.

For the Future:

- General reformulation of FLT for arbitrary Fermi surface geometry and topology. Bosonization revisited? Use differential geometry of manifolds
- non-Abelian SO(3) Berry effects on spin-degenerate Fermi surface?
- role of "quantum distance" ? (approach weak localization by adding disorder to FLT, not interactions to disordered free electrons?)
- wormholes (monopoles at band degeneracies) and other exotica! (singular Berry curvature means a singular metric)