Attachment of Surface “Fermi Arcs” to the Bulk Fermi Surface: “Fermi-Level Plumbing” in Topological Metals

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The role of “Fermi arc” surface-quasiparticle states in “topological metals” (where some Fermi surface sheets have non-zero Chern number) is examined. They act as “Fermi-level plumbing” conduits that transfer quasiparticles among groups of apparently-disconnected Fermi sheets with non-zero Chern numbers to maintain equality of their chemical potentials, which is required by gauge invariance. Fermi arcs have a chiral tangential attachment to the surface projections of sheets of the bulk Fermi Surface: the total Chern number of each projection equals the net chirality of arc-attachments to it. Information from the Fermi arcs is needed to unambiguously determine the quantized part of the anomalous Hall effect that is not determined at the bulk Fermi surface.

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The recent interest in “Weyl semimetals” and the topological “Fermi arc” states on their surfaces[1] raises the question of how these evolve as the Fermi level moves away from the semimetal point, and metallic behavior is restored. If the Weyl semimetal has broken time-reversal symmetry, it exhibits an unquantized intrinsic anomalous Hall effect (AHE), which can be obtained as a limiting case of the general Fermi-surface formula[2] for the unquantized part of the intrinsic AHE of the metal. The Weyl-semimetal surface-state Fermi arcs survive in the metallic state as “surface conduits” that can adiabatically transfer quasiparticles between topologically-non-trivial sheets of the metallic Fermi surface (FS) that are disjoint in the bulk. In this Letter, I will show how they are related to, and required by, topological features of the Fermi surface AHE formula[2].

The Karplus and Luttinger “intrinsic” theory[3] of the AHE in ferromagnetic metals was largely ignored until it was reinterpreted[4, 5] in modern language in terms of the geometrical (Abelian) Berry curvature of the spin-split Bloch bands, and is now recognized as a major component of the AHE (in addition to “extrinsic” terms). In agreement with the fundamental notion that all transport processes occur at the Fermi level, it was subsequently shown[2] that Karplus and Luttinger’s AHE formula could be expressed (up to a topologically-quantized part) in terms of Fermi-surface geometry in the Brillouin zone (BZ), plus the Berry-connection geometry of quasiparticle states at the FS. Note that, within Fermi-liquid theory, the infinite-lifetime quasiparticle states at the $T = 0$ Fermi level are the only non-topological features of one-electron band theory that completely survive in the presence of interactions.

The intrinsic AHE Fermi-surface formula for a 3D metal with broken time-reversal symmetry states that the intrinsic Hall conductivity tensor has the form

$$\sigma_H^{ab} = \frac{e^{abc} K^H_c}{2\pi R_K}, \quad (1)$$

where $R_K = e^2/h$ is the fundamental quantum unit of electrical resistance, and $K^H$ is a reciprocal vector with units [length]$^{-1}$. If a uniform magnetic flux density $B$ passes through a finite sample with volume $V$, held at fixed electronic chemical potential $\mu$, the total electronic charge $Q$ obeys the Strøeda relation

$$\lim_{V \to \infty} \frac{1}{V} \frac{\partial Q}{\partial B^0} = \frac{K^H_0}{2\pi R_K}. \quad (2)$$

This relation requires the existence of states at the Fermi level if $K^H \neq 0$ (which may be surface states).

If the bulk material in the limit $T \to 0$ is an insulator with no Fermi surface, $K^H = G \in \Lambda$, the Bravais lattice of reciprocal lattice (Bragg) vectors of the bulk crystal structure. If $G = \nu G_0$, where $\nu$ is an integer, and $G_0$ is primitive, this is equivalent to a 2D integer quantum Hall effect $\sigma_H = \nu R_K^{-1}$ in each lattice plane indexed by $G_0$. From a band-structure perspective, $G = G_{QHE} = \sum_i G_i$, where $G_i$ are topological invariants (an integral of the Berry curvature) of each disjoint group of occupied bulk bands below the Fermi level, but it is also a Fermi-level property of topologically-required surface states on facets of a crystal not normal to $G_{QHE}$.

If a system with no bulk states at the Fermi level has $K^H$ quantized as a reciprocal lattice vector, the non-quantized part of $K^H$ must be a bulk Fermi-surface property[2]. It will be here assumed that the (spin-split) FS is “regular”, i.e., everywhere non-degenerate, with a finite Fermi velocity, and described by a set of disjoint differentiable orientable 2-manifolds $\{S_i\}$ embedded in the (reduced) 3D BZ. This is the generic case for a ferromagnetic metal.

A FS sheet may be parameterized by $s = (s^1, s^2)$, with an area 2-form “$d^2 S \equiv ds^1 \wedge ds^2$”, and $n_F$ is the outward normal (direction of the Fermi velocity). The full AHE formula[2] is

$$K^H = G + \sum_i \int_{S_i} \frac{k_F}{2\pi} + \sum_{\alpha} \oint_{\partial S_{i\alpha}} \frac{G_{i\alpha}A}{2\pi}. \quad (3)$$
Here $\mathcal{F}$ is the Berry-curvature 2-form $\frac{1}{2}e_{abc}n^a_F \mathcal{F}^{bc} dA$ where $\mathcal{F}^{ab} = \nabla^a A^b - \nabla^b A^a$ is the Bloch-state Berry curvature, expressed in terms of the Berry connection $A^a$. The quantity $A^a dk_n$ is the Berry-connection 1-form on curves $\partial S_{i\alpha}$ where sheet $S_i$ of the FS intersects the “reduced BZ boundary” (see below). Note that, in the language of differential forms, $\mathcal{F}$ is the exterior derivative $dA$.

It is perhaps useful to note that the Bloch-state Berry connection $A^a_n(k) = -i\langle \Phi_n(k)|\nabla^a|\Phi_n(k)\rangle$ is defined not just by the Bloch states $|\Psi_n(k)\rangle$ themselves, but by $|\Phi_n(k)\rangle = U(-k)|\Psi_n(k)\rangle$, with

$$U(k) = \sum_{R_\alpha} \exp(i\mathbf{k} \cdot \mathbf{x}_{R_\alpha})|\mathbf{R}, \alpha\rangle \langle \mathbf{R}, \alpha|,$$  

(4)

where $|\mathbf{R}, \alpha\rangle$ is an orthonormal basis of spatially-localized orbitals in unit cell $\mathbf{R}$, that is embedded in Euclidean space at $\mathbf{x}_{R_\alpha} = \mathbf{R} + \mathbf{x}_\alpha$, so the Berry curvature of Bloch states depends not only on the details of the electronic band structure, but also on the location of orbitals within the unit cell. This affects the semiclassical equations of motion [3, 4], but not the topological invariants.

While the coordinate-independent formula [3] is a simple and elegant expression, it has a number of subtleties. First, I note that the Bloch vector $\mathbf{k}$ (and hence the quasiparticle Fermi vector $\mathbf{k}_F$) of a charged particle is itself ambiguous when time-reversal symmetry is broken, as under a gauge-transformation, $k \rightarrow k - eA/h$, $\nabla \times A = 0$. In particular, the choice of a constant vector potential $A$ is compatible with Bloch states, and can only be excluded if time-reversal symmetry is unbroken. All physically-meaningful (i.e., gauge invariant) formulas should therefore be invariant under the mapping $\mathbf{k}_F \rightarrow \mathbf{k}_F + \text{constant}$. Thus gauge invariance imposes the condition

$$\sum_i \int_{S_i} \mathcal{F} = \sum_i c_1(S_i) = 0,$$  

(5)

where the integer $c_1(S_i)$ is the “Chern number” of Fermi-surface sheet $S_i$ (more technically, the first Chern class of the mapping between the 2-manifold $S_i$ and the “$U(1)$ fiber bundle” defined by the $\mathbf{k}_F$-dependent quasiparticle wavefunctions inside the unit cell).

While the reciprocal-vector-valued 1-form $dk_F$ is well-defined, the reduction of $\mathbf{k}_F$ to the reduced BZ (which formally is a 3-torus with a Euclidean metric) means that if a Fermi-surface sheet $S_i$ admits “open orbits” where

$$\oint_{S_i} dk_F = G(\Gamma) \neq 0,$$  

(6)

it is necessary for it to contain inscribed boundary lines $\partial S_{i\alpha}$ across which $\mathbf{k}_F$ jumps by a reciprocal vector $G_{i\alpha}$. Then $G(\Gamma) = -\sum_{\alpha} G_{i\alpha}$ is canceled by the sum of jumps along the path $\Gamma$. With the inscribed boundaries, Stokes’ theorem can be used to write $\int_{S_i} k_F \mathcal{F} = \int_{S_i} k_F dA$ as an integral over the interior of the intersection of $S_i$ with the reduced BZ, plus boundary terms. The boundary terms come in matched pairs $\partial \Sigma_{i\alpha \pm}$, which combine to give the second term in [3] (The version of [3] given in Ref. [2] sums over both “+” and “−” boundaries, so has a prefactor $1/4\pi$ in front of the second term; since these are two sides of the same boundary, and contribute equal amounts, they have here been combined into a single term in [3]). The choice of the BZ boundaries on each $S_i$ is a completely-arbitrary “gauge choice”, so physically-meaningful results must be invariant under a continuous change of $\partial S_{i\alpha}$: the formula [3] satisfies this requirement.

The embeddings of bulk FS sheets in the BZ also have some topological characteristics that are independent of Berry curvature. While not directly relevant to the AHE, I list them here for completeness. The set of open-orbits define a Bravais lattice $\tilde{\Lambda}_i = \{G(\Gamma), \Gamma \in S_i\} \subset \tilde{\Lambda}$. The Gauss-Bonnet theorem relates the integral of the Gaussian-curvature 2-form $\kappa = \frac{1}{2} \epsilon_{abc}a^a \partial_a n_F \times \partial_b n_F dS^a \wedge dS^b$ to the genus. Finally, “Quasi-1D” systems are characterized by a special primitive lattice translation $\mathbf{R}_0$, where all open orbits have $G(\Gamma) \cdot \mathbf{R}_0 = 0$, and some FS sheets have a “Luttinger anomaly” (chiral anomaly)

$$2\pi \int_{S_i} n_F dA = \Omega_{\text{BZ}} \sigma_i \mathbf{R}_0, \quad \sigma_i = \pm 1,$$  

(7)

where $\Omega_{\text{BZ}}$ is the reciprocal-space volume of the BZ. Such FS sheets do not enclose a definite reciprocal-space volume, so the Luttinger theorem (relating the geometric volume of the Fermi surface to electron density) does not apply to them individually. Gauge invariance requires that the total Luttinger anomaly $\sum_i \sigma_i$ vanishes.

The gauge-invariance conditions can be strengthened in the “ultra-clean” limit where equilibration of the Fermi surfaces only occurs through scattering processes with infinitesimal momentum transfer. In that limit, a separate chemical potential can be established on disjoint FS sheets $S_i$, which gain separately-conserved quasiparticle currents. This requires invariance of the AHE formula [3] under a rigid displacement of $\mathbf{k}_F(s)$ (a gauge transformation) for the sheet $S_i$ by itself. Only sets of sheets with zero total Chern number can be displaced together to define such conserved currents.

Each conserved quasiparticle current will be associated with an independent chemical potential, so “irreducible sets” of FS sheets associated with a common chemical potential can be defined. In the simplest case, a sheet with Chern number $+1$ is paired with a partner that has Chern number $-1$. (The systematic classification of the possible structures of “irreducible sets” of FS sheets is left as an open problem.) The members of such a pair maintain a common chemical potential, so slowly-varying external fields must be able to “pump” quasiparticle charge between them without any quasiparticles being scattering through the regions of reciprocal space that separate the disjoint members of the pair in the BZ. Ref. [2] attributed...
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The recent work on Weyl semimetals [11] allows the

mechanism for maintaining a common chemical potential.

In Weyl semimetals, the Fermi surface collapses to a set

of discrete points in the BZ, which are band-touching
degeneracies. The Weyl points at $k_{i}^{0}$ are monopole sources

of “Berry flux” which absorb a multiple of $2\pi$ of Berry
curvature flux from one band, and emit it into the other.

If the Fermi level is slightly shifted above or below the

Weyl points, regular Fermi surfaces surrounding each

Weyl point emerge, with Chern numbers $c_{i}(S_{i}) \equiv c_{i}$.

The limit of $K^{H}$ as the Fermi level passes through the

Weyl points is just

$$K^{H} = G + \sum_{i} c_{i}k_{i}^{H}. \quad (8)$$

A simple “toy model” for the Fermi arc is provided by a 1D model often used to model a “quantum pump”:

$$H = \sum_{n=1}^{\infty} (-1)^{n} V c_{n}^{\dagger} c_{n} + \sum_{n, \pm} (t_{n+} c_{2n+1}^{\dagger} c_{2n} + \text{H.c.}). \quad (9)$$

The two bulk bands are $\varepsilon_{\pm}(k) = \pm \sqrt{(V^{2} + t_{+}^{2} + t_{-}^{2} +

2 t_{+} t_{-} \cos k)}$. I will take $t_{+} > 0$; the band gap then
closes at $k = \pi$ for $t_{+} = t_{-}$. In general, the gap is $|E| < \sqrt{(V^{2} + (t_{+} - t_{-})^{2})}$, and for $|t_{-}| < t_{+}$, there is an edge-state in the gap with $\Psi_{2n} = 0$, $\Psi_{2n+1} = (t_{-}/t_{+})^{n}\Psi_{1}$, and $E = V$. By making $V$, $t_{-}$ and $t_{+}$ functions of the surface Bloch vector $k = (k_{x}, k_{y})$, this can model Weyl points and their Fermi arcs [10].

As an example, Fig. (1) shows results for model parameters $(V, t_{-}, t_{+}) = (k_{y}, |k|, 1)$ The surface state has dispersion $E(k) = k_{y}$, and exists for $|k| < 1$, and its decay length into the bulk diverges as $|k| \to 1$. For Fermi energy $E_{F} = 0$, the model is a Weyl semimetal with Weyl points at $k = (\pm 1, 0)$. For $E_{F} \neq 0$, the boundaries of the region of the projected bulk FS are given by

$$(k_{y})^{2} + (|k| - 1)^{2} = (E_{F})^{2}, \quad (10)$$

and shown in Fig. (1) for selected values of $E_{F}$. For $|E_{F}| < 1$ a Fermi arc of 2D quasiparticles connects two points on the surface of the projected FS, and emanates tangentially from it.

The “toy model” highlights a number of features. First, its surface states are an “incomplete band”, as they exist in only a limited region of $k$-space, and would not cover the full two-dimensional surface BZ (2DBZ) in a realistic model that was periodic parallel to a crystal facet. Instead, the surface band terminates on a $k$-space boundary at which the decay-length into the bulk diverges. Close to the boundary, the surface state is extremely weakly-bound, and its properties approach those of the bulk electronic band from which it evolves at the termination point. In particular, its group velocity tangent to the surface will approach that of the bulk band edge at the termination point from which it evolves.

The end points of Fermi arcs are at the intersection of the projected bulk FS with the termination line where an incomplete surface band leaks into the bulk, and the attachment is thus generically tangential. In the 2DBZ, the Fermi-vector 1-form $dk_{F}$ can be given a standard direction so that $n \times v_{F} \cdot dk_{F} > 0$, where $n$ is the outward normal of the facet, and $v_{F}$ is the surface quasiparticle Fermi velocity tangent to the facet. At the attachment point $k_{i}$, there are two possible tangential directions for the arc to leave the attachment point: $\xi_{i}dk_{F}$ where $\xi_{i} = \pm 1$. By inspection, there a sum rule

$$\sum_{i \in P_{FS}} \xi_{i} = \sum_{i \in P_{FS}} c_{i}(S_{i}) \quad (11)$$

where the LHS is the the sum of attachment chiralities to a given region $P_{FS}$ of projected FS in the facet BZ, and the RHS is the sum of Chern numbers of the bulk FS sheets contributing to the projection. If this is non-zero, a net number of directed Fermi arcs flow towards or away from $P_{FS}$, and must terminate on other projections with compensating Chern numbers.

There is no need for a projected FS to have a topologically-non-trivial Chern number for it to be attached to a Fermi arc, as the “toy model” shows for $1/\sqrt{2} < |E_{F}| < 1$. Arcs that detach and re-attach to the same FS projection do not affect the LHS of (11).

The arcs define a 1D open manifold of surface quasiparticle states embedded in the facet 2DBZ. Closed surface quasi-particle manifolds $C_{i}$ (unconnected to the Bulk FS
the closed directed Fermi curve $C_\alpha$ where thus (on a clean surface) support independent chemical potentials, justifying the additional surface term they contribute in (13). In contrast, the 2D AHE formula of Ref.\cite{2} has no obvious place for a contribution to the subleading surface-AHE from open Fermi arcs, since only closed 1-manifolds can have a gauge-invariant Berry phase factor $\exp i \oint A$. In addition, the Fermi arcs do not have chemical potentials independent of the bulk FS sheets they attach to, so it seems consistent that, as well as not contributing to the non-quantized part of the bulk AHE (in contradiction to recent claims\cite{11}), they will also not contribute any independent extra non-quantized terms to the sub-leading (facet) terms of (13).

As a final example, consider a system which has a trivial insulator bulk with $K = 0$, and where all facets are 2D Chern insulators. In this cases the only states at the Fermi level are chiral 1D Fermi liquids on the edges of the facets, which form a network of 1D edges, each of which has a directed integer chiral anomaly $\nu$. The edges are joined at the crystal vertices, and the net outgoing chiral anomaly on edges leaving a vertex must vanish. This means that the formula (13) has the correct form, as it can then be decomposed into a sum of facet terms, each of which contributes an quantized integer QHE term $\nu_\alpha A_\alpha n_\alpha^\alpha / R_K$ to (13). The absolute value of $\nu_\alpha$ is determined on each edge by the chiral anomaly, the number of “right-moving” minus the number of “left moving” Fermi points, which can each have its own chemical potential.

The preceding discussion assumes that the Fermi surfaces in the 3D BZ, as well as the closed Fermi curves and open Fermi arcs in the facet 2DBZ, are described by Fermi-liquid theory. In the final example, where the only gapless excitations derive from integer quantum Hall edge states on the crystal edges between facets, there is a natural interaction-based generalization to fractional quantum Hall states, with fractional Chern insulator facets. An interesting open question remains: can the gapless 2D or 3D Fermi-liquid states, which provide non-quantized geometric parts of the formula (13), also have non-trivial generalizations in strongly-interacting systems?

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