Orbital magnetization, geometric phase, and a modern theory of magnetic breakdown

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Semiclassical theory of Bloch electrons in a magnetic field

A method to calculate wavefunctions and energy levels which become increasingly accurate in the limit that a **classical action function** (A) becomes much larger than a parameter characteristic of the field.

Hamilton’s equation

\[ \dot{k} = -\frac{e}{c} \nabla_k \varepsilon \times B \]

Semiclassics hold when the area of orbit

\[ A \gg l^{-2} = \frac{eB}{\hbar c} \]

inverse square of magnetic length

example: closed orbit
Modern notions in the semiclassical theory
developed in wavepacket and effective-Hamitonian theory
(Chang, Sundaram et al, Qian Niu, Culcer et al)
(Roth, Blount, Kohn)

Geometric phase

Berry phase
\[ \exp \left( i \int \mathcal{X} \cdot dk \right) \]

For a pseudospin-half \( H(k) = R(k) \cdot \sigma \),
the Berry phase is half the solid angle
subtended by the three-vector \( R(k) \).

If a symmetry enforces \( R(k) \) to lie in a plane,
the solid angle is \( 2\pi \).
Orbital magnetic moment in atoms

Correction to groundstate energy

\[ \Delta E = \mu_B B \cdot \langle 0 | L | 0 \rangle \]

\[ L = \sum_i r_i \times p_i \]

If \( |0\rangle \) is nondegenerate, then time-reversal symmetry enforces \( \Delta E = 0 \).

Orbital magnetic moment in solids

orbital angular momentum of a wavepacket rotating about its center of mass

\[ |W(r)|^2 \]

(C Chang, Niu, PRB 53, 7010)

Correction to energy of wavepacket \( |w\rangle \)

\[ \Delta E = \mu_B B \cdot \langle w | (r - r_c) \times p | w \rangle \]

T-invariant solids can have nonzero orbital magnetization owing to its action on the crystal momentum

\( T: k \rightarrow -k \)
These modern notions refine the Bohr-Sommerfeld quantization conditions.

**Review of traditional Bohr-Sommerfeld**

Onsager-Lifshitz: \( l^2 A(E_n) = \pi(2n + 1) \quad n \in \mathbb{Z} \quad l^{-2} = eB/\hbar c \)

For fixed field \( B \), discrete energetic solutions are Landau levels.

Maslov correction: ‘Zero-point energy from quantum fluctuations’

Ex. Schrödinger \( \varepsilon = (k_x^2 + k_y^2)/2m \)

\( A(E) = \pi(k_x^2 + k_y^2) = 2\pi m E \)

\[
\frac{2\pi}{l^2 m} = \frac{2\pi}{l^2 (dA/dE)}
\]

Effective mass \( = dA/dE \)
At fixed Fermi energy, $l_n^2$ are values of the inverse fields where Landau levels successively become equal to the Fermi energy.

$$l_n^2 A(E_F) = \pi (2n + 1)$$

$$l_{n+1}^2 - l_n^2 = 2\pi / A(E_F)$$

leads to dHvA oscillations.

First observation in Bismuth de Haas, van Alphen (1930)

Phenomenology of relating magnetic phenomenon the shape of the Fermi surface: ‘Fermiology’ of metals

Relate magnetic phenomenon to robust properties of the Fermi-surface wavefunction: ‘Topo-Fermiology’
Infinite-field intercept of dHvA oscillations

Onsager-Lifshitz: \( l_0^2 A(E_F) = \pi \) \( \gamma \)-intercept
Maslov

Ex. 1: Schrodinger

Ex. 2: Dirac

To find a Dirac point without ever seeing it.

Standard lore for nondegenerate band

\[
\gamma \text{-intercept} = \pi + \begin{cases} 
0, & \text{Schrodinger} \\
\pi, & \text{Dirac} 
\end{cases}
\]

(Berry,Mikitik PRL 82 2147)
For D-fold degenerate bands, (e.g., D=2: spin-degeneracy)

\[ l^2 A(E) = 2\pi n + \pi - \lambda_\alpha \]

\( \alpha = 1, \ldots, D \)

\( \{\lambda_\alpha\} \) encodes the modern corrections

(i) orbital magnetization (vanishes in centrosymmetric metals without SOC)
(ii) the geometric phase (non-abelian for D>1, and generally a continuous quantity).

At fixed \( l^2 \), solutions \( (E_{n,\alpha}) \) correspond to D sets of sub-Landau levels.

At fixed \( E \), solutions \( (l^2_{n,\alpha}) \) correspond to D sub-harmonics in the dHvA; each sub-harmonic has its own intercept \( \gamma_\alpha = \pi - \lambda_\alpha \).

Our contribution:
(a) gauge-independent formulation of \( \{\lambda_\alpha\} \) for multi-band quantization rule
   (Gauge-dependent formulations for D=2 by Roth, Mikitik)
(b) symmetry analysis determines in which solids, and for which field orientation,
   - is the Berry phase discrete/continuous?
   - is the orbital moment nonvanishing?
   - is \( \gamma_\alpha/\pi \) rational and robust to Hamiltonian deformations?

\( \gamma_\alpha/\pi \) are the topological invariants in magnetotransport.
Can the modern semiclassical concepts be combined with quantum tunneling?

Beyond semiclassical theory

Magnetic breakdown

(Cohen, Falicov, Blount, Pippard, Azbel, Chambers, Slutskin)

The geometric phase and orbital moment are quantities defined on orbits.

Semiclassical orbits are no longer well-defined in the presence of quantum tunneling.

Can the modern semiclassical concepts be combined with quantum tunneling?

Modern theory of magnetic breakdown

Our contribution:
Generalized Bohr-Sommerfeld quantization conditions that are beyond semiclassical, i.e., they incorporate GP, OM and MB.

Analytic, quantitative understanding of magnetic energy levels and dHvA peaks.
Many topological bandstructures, with unremovable geometric phase, unavoidably undergo breakdown.

Surface states of topological insulators

Hourglass fermions
(AA, Z. Wang, Bernevig, prx 6, 021008)

SnTe
(T. Hsieh, L. Fu, Nat. Comm 3:982)

Topological metals

Tilted Dirac/Weyl fermion
(Soluyanov, Bernevig, Nature 527, 495; Isobe, PRL 116, 116803; Muechler, AA, Neupert, Car PRX 6, 041069)
Outline

Effective Hamiltonian of a Bloch electron in a magnetic field

Bohr-Sommerfeld quantization conditions for closed orbits.

Symmetry analysis of the quantization condition.
Formulate topological invariants in magnetic transport.

Quantization conditions that incorporate breakdown.
Effective Hamiltonian of a Bloch electron in a magnetic field

(Peierls, Luttinger, Wannier, Fredkin, Roth, Blount, Kohn, Zak, Nenciu)

Aim: describe dynamics within a low-energy subspace spanned by \( D \) degenerate bands.

Solution: identify a good quantum-mechanical representation, i.e., basis functions.

\[ \phi_{nk}(r) = e^{ik \cdot r} \psi_{n,k+a(r)}(r) \]

Field-modified Bloch functions form a representation of magnetic translations

(Brown, Zak, Misra)

\[ (\hat{H} - E)\psi = 0 \quad \psi(r) = \sum_{nk} g_{nk} \phi_{nk}(r) \]

\[ \sum_{n=1}^{D} (\mathcal{H}(K)_{mn} - E \delta_{mn}) g_{nk} = 0 \]

\( \mathcal{H}(K) \), the effective Hamiltonian, is a symmetrized function of the kinematic quasimomentum operator:

\[ K = k + a(i\nabla_k) \quad K \times K = -i\frac{e}{c} B \]
\[ \mathcal{H}(\mathbf{K}) = H_0(\mathbf{K}) + H_1(\mathbf{K}) + H_2(\mathbf{K}) + \ldots \quad H_j(\mathbf{k}) = \mathcal{O}(B^j) \]

\[ H_0(\mathbf{k}) = \varepsilon_n \mathbf{k} \quad \text{Peierls-Onsager Hamiltonian} \]

To leading order in $B$, dynamics occurs within the low-energy subspace.

To next order in $B$, interband transitions occur between low- and high-energy subspaces.
Beyond the Peierls-Onsager theory  
(Roth, Blount, Kohn)

\[ H_1(k) = H_1^B + H_1^{OM} + H_1^Z \]

generates the **Berry** phase  \( B \times \text{orbital moment} \) **Zeeman** coupling

\[
\exp \left( -i \oint H_1^B \, dt \right) = \exp \left( i \oint \mathbf{A} \cdot \, dk \right) \\
\mathbf{A}(k)_{mn} = i \langle u_{m,k} | \nabla_k u_{n,k} \rangle
\]

\[ H_1^{OM} = \mu_B \mathbf{B} \cdot \mathbf{r}_{\text{off}} \times \mathbf{p}_{\text{off}} \quad \text{(off-diagonal w.r.t. to low- and high-energy subspaces)} \]

\[ = \mu_B B \sum_{\tilde{m} \neq n} i \langle u_{m,k} | \nabla_k x \tilde{u}_{m,k} \rangle \langle \tilde{u}_{m,k} | \hat{p}^y | u_{n,k} \rangle - (x \leftrightarrow y) \]

Terms analogous to \( H_1^B \) and \( H_1^{OM} \) appear ubiquitously in the asymptotic theory of coupled wave equations  
(Littlejohn, Flynn, PRA 44, 5239)
The effective Hamiltonian does not depend on its basis in the usual way.

\[ |u_{nk}\rangle \rightarrow \sum_{m=1}^{D} |u_{mk}\rangle V_{mn}(k), \quad V^{-1} = V^{\dagger} \]

What we have shown:

For Chern insulators with short-ranged hoppings,

\[ H_1 \not\sim V^{-1}H_1V. \]

For symmetry-protected topological insulators, \( H_1 \) transforms anomalously under symmetry.

The theory of effective Hamiltonians is fundamentally a gauge theory.

Basic gauge-covariant objects: ‘Wilson loops’

\[ \mathcal{P} \exp (-i \int H_1 dt) \rightarrow V^{-1} \mathcal{P} \exp (-i \int H_1 dt) V \]

Gauge-invariant eigenvalues \( \{ e^{i\lambda_a} \} \) enter the quantization condition.
Wilson loops appear in the WKB wavefunction of effective Hamiltonians

\[
\left( H_0(K) + H_1(K) - E \right) g(k) = 0 \quad K_x = k_x + il^{-2}\partial_y, \quad K_y = k_y
\]

vector wavefunction \( \mathcal{P} \exp \left( -il^2 \int (k_x - H_1(\frac{\partial \varepsilon}{\partial k_x})^{-1}) dk_y \right) * g(0) \)

Quantities in the exponent are evaluated on the band contour.

(Generalizes single-band wavefunction by Zilberman, Fischbeck)

sweeps out the area \( \mathcal{A} \) of the circle

generates the propagator \( \mathcal{P} \exp (-i \int H_1 dt) \)

with eigenvalues \( \{e^{i\lambda_\alpha}\} \)

\( \alpha = 1, \ldots, D \)

Quantization condition for closed orbits is equivalent to imposing continuity of (vector) wavefunction around a loop

\[
l^2 A = 2\pi n - \lambda_\alpha + \pi
\]

Maslov
\[ l^2 A = 2\pi n - \lambda_a + \pi \]

dHvA intercepts \[ \gamma_a = -\lambda_a + \pi \] (±\(\pi/4\) Lifshitz-Kosevich correction in 3D)

In some solids, and for certain field orientations, \[ \lambda_a/\pi \] (and hence \[ \gamma_a/\pi \])
is symmetry-fixed to a rational number.

\[ \gamma_a \] are the topological invariants of magnetotransport.

Case studies: graphene, Bi2Se3, 3D Weyl metals (WTe2), SnTe, WSe2

Role of symmetry and field orientation in rationalizing \[ \gamma_a/\pi \].
### Spacetime-inversion symmetry:

Like a time-reversal symmetry that maps \( \mathbf{k} \rightarrow -\mathbf{k} \)

Sublattice pseudospin lies in plane:

Berry phase of pi,

Orbital magnetization is suppressed.

\[ \gamma = 0 \]

---

### 2D spinless Dirac point

(ex: Graphene)

[Diagram of hexagonal lattice with arrows for pseudospins]

### 2D spinful Dirac point

(ex: surface of Bi2Se3)

[Diagram with crossing arrows for \( k_x \) and \( k_y \) and Berry phase symbol]
Time-reversal-related massive Dirac fermions

Spinless graphene with broken spatial-inversion symmetry: no $k \rightarrow k$ constraint.

Due to T symmetry acting as $k \rightarrow -k$, pseudospins on different orbits cant in opposite directions.

Each valley-centered orbit produces a dHvA harmonic, and the two intercepts are symmetry related: $\gamma_1 = -\gamma_2$. 
2D solids: $\gamma/\pi$ deviates from rationality when a spatial symmetry is broken.

3D solids: one can change the symmetry of the extremal orbit (and hence $\gamma$) by tilting the field with respect to a crystal axis.

High-symmetry plane invariant under two-fold rotation and time reversal

Weyl fermion centered on a generic wavevector on the plane. (e.g., strained WTe2, Soluyanov et al)

Symmetric extremal orbit $\lambda = \pi$, $\gamma = -\pi/4$

Asymmetric extremal orbit $\gamma \neq -\pi/4$
For which solids and field orientations are \( \lambda_a/\pi \) (and hence \( \gamma_a/\pi \)) symmetry-fixed to rationality?

10 (and only 10) classes of closed, symmetric orbits. Each class corresponds to a unique group algebra for the propagator

\[
\mathcal{A} = \mathcal{P} \exp \left( -i \int H_1 dt \right)
\]

Constraints on \( \lambda_a \) are derived from this algebra.

<table>
<thead>
<tr>
<th>( u )</th>
<th>( s )</th>
<th>Algebra</th>
<th>Representation</th>
</tr>
</thead>
<tbody>
<tr>
<td>(I) ( \forall k^\perp ), ( k^\perp = g \circ k^\perp )</td>
<td>0 0</td>
<td>( \mathcal{A} = \bar{g} \mathcal{A} \bar{g}^{-1} )</td>
<td>( \bar{g}^2 = e^{i \pi F_a - i k \cdot R} )</td>
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<td></td>
<td>0 1</td>
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<td>=</td>
<td>g \circ \mathcal{O}</td>
</tr>
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<td></td>
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<td>( \mathcal{A} = \bar{g} \mathcal{A}^* \bar{g}^{-1} )</td>
<td>( (\bar{g} K)^2 = A^{\pm} N/L e^{i \pi F_a} )</td>
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<td></td>
<td>1 0</td>
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<td>1 1</td>
<td>( \mathcal{A} = \bar{g} \mathcal{A}^t \bar{g}^{-1} )</td>
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</tr>
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<td>\neq</td>
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<td></td>
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<td>( \mathcal{A}_{i+1} = \bar{g}_i \mathcal{A}_i^* \bar{g}_i^{-1} )</td>
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</table>

Rational
Rational
Landau-level degeneracy
Symmetric splitting
Symmetric splitting
Landau-level degeneracy
Why only 10 classes of symmetric orbits?

For any symmetry \( g \), three distinct types of mappings in 2D \( k \)-space:

Class I: \( k \rightarrow k \)

Class II: \( k \rightarrow g \circ k \neq k \)

Class II-A: \( k \) and \( g \circ k \) lie on the same orbit

Class II-B: \( k \) and \( g \circ k \) on distinct orbits

\( u = 0 \) (orientation-preserving), \( 1 \) (reflection)

\( s = 1 \) (includes time reversal), \( 0 \) (purely spatial transformation)

<table>
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<tr>
<th>Class</th>
<th>( k )-space</th>
<th>Surface</th>
<th>Description</th>
<th>( \lambda )</th>
</tr>
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<tr>
<td>(I)</td>
<td>( \forall k^\perp, k^\perp = g \circ k^\perp )</td>
<td>Graphene</td>
<td>Rational</td>
<td>( \lambda )</td>
</tr>
<tr>
<td>(II-A)</td>
<td>( k^\perp \in o,</td>
<td>Surface of Bi2Se3</td>
<td>Rational</td>
<td>( e^{i \sum_a \lambda_a} \in \mathbb{R} )</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Surface of SnTe</td>
<td></td>
<td></td>
</tr>
<tr>
<td>(II-B)</td>
<td>( k^\perp \in o,</td>
<td>Bilayer graphene</td>
<td>Landau-level degeneracy</td>
<td>{\lambda_a^{i+1}} = {\lambda_a^i}</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Deformed graphene, WSe2</td>
<td>Symmetric splitting</td>
<td>{\lambda_a^{i+1}} = {-\lambda_a^i}</td>
</tr>
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\( \lambda \) represents the eigenvalues of the system under the given symmetry transformations.
Magnetic breakdown
(Cohen, Falicov, Blount, Pippard, Azbel, Chambers, Slutskin)

Within the breakdown region, band contours approach each other hyperbolically.

Dimensionless parameter in breakdown region
\[ \mu \propto abl^2 \]

Breakdown is insignificant if
\[ |\mu| \gg 1 \]
The orientation of travelling wavepackets distinguish two qualitatively distinct types of breakdown.

**Intraband breakdown**

Two contours belong to the same band.

The saddlepoint is the nucleus of Lifshitz transitions.

**Interband breakdown**

The two contours belong to different bands.

Line nodes in 3D metals.
Over-tilted Weyl/Dirac points.

Hourglass fermion
KHgSb
Goals

Magnetic energy levels and dHvA peaks are determined by generalized Bohr-Sommerfeld quantization rules that unify tunneling, geometric phase and the orbital moment.

Formulate topological invariant that:
(i) non-perturbatively encodes quantum tunneling,
(ii) distinguishes metals with differing Berry phases on their Fermi surface.
A Schrödinger particle with $\hbar = l^{-2}$, coordinate $= k_y$.

At zero energy ($\mu = 0$),

$$|\mathcal{R}|^2 = |\mathcal{T}|^2 = 1/2 \quad \text{(Kemble)}$$

Semiclassics ‘breaks down’

$$\dot{k} = \frac{e}{c} \nabla_k \varepsilon \times B \to 0$$

A hypothetical wavepacket never reaches the saddlepoint in finite time.
Two orbits merge into one.

Analogy: double well

Conventional metal

Topological metal
near a metal-insulator phase transition

ex: strained graphene

Two orbits merge into one.

Analogy: double well

Conventional metal

Topological metal
near a metal-insulator phase transition

ex: strained graphene
Quantization condition

\[
\cos\left(\frac{\Omega_1 + \Omega_2}{2} + \text{phase}(\mathcal{T})\right) = |\mathcal{T}| \cos\left(\frac{\Omega_1 - \Omega_2}{2}\right)
\]

\[\mathcal{T} = \frac{e^{\pi \mu / 2}}{\sqrt{2 \cosh(\pi \mu)}} e^{i \arg[\Gamma(1/2-i\mu)] + \mu \log |\mu| - \mu}\]

\(\Omega_1 = \) semiclassical phase acquired by wavepacket around a closed Feynman trajectory.

\[\Omega_j = -l^2 A_j(E) + \pi + \varphi_B\]

\(\varphi_B = \begin{cases} 0, & \text{(conventional)} \\ \pi, & \text{(topological)} \end{cases}\)

Continuity of wavefunction of the effective Hamiltonian:

\[
\det \left[ \begin{pmatrix} \mathcal{T} & \mathcal{R} \\ \mathcal{R} & \mathcal{T} \end{pmatrix} \begin{pmatrix} e^{i\Omega_1} & 0 \\ 0 & e^{i\Omega_2} \end{pmatrix} - I \right] = 0
\]

Scattering matrix

Semiclassical evolution
Quantization condition

\[ \cos \left( \frac{\Omega_1 + \Omega_2}{2} + \text{phase}(\mathcal{T}) \right) = |\mathcal{T}| \cos \left( \frac{\Omega_1 - \Omega_2}{2} \right) \]

Two independent orbits
\[ \Omega_j = 2\pi \mathbb{Z} \]
\[ = -t^2 A_j(E) + \pi + \varphi_B \]

A single enlarged orbit
\[ \Omega_1 + \Omega_2 = 2\pi (\mathbb{Z} + 1/2) \]

Incommensurate harmonics \((\Omega_1 \pm \Omega_2)/2 \rightarrow \text{quasirandom}\) spectrum

Level spacings are not equidistant, but exhibit long-range correlations.

Typical spectrum

\[ \mathcal{T} \approx 0 \]

Dominant harmonic \((\Omega_1 + \Omega_2)/2\) determines semiclassical Landau fan.

Leading-order tunneling correction oscillates with the frequency of \((\Omega_1 - \Omega_2)/2\).

We develop a perturbation theory for quasirandom spectra:

\[ \delta E_j = \frac{\text{phase}(\mathcal{T}) + (-1)^j |\mathcal{T}| \cos \left( \frac{\Omega_1 - \Omega_2}{2} \right)}{-\frac{1}{2} \partial(\Omega_1 + \Omega_2)/\partial E} \]
Symmetry restores commensurability

2D Dirac points are stabilized by spatial-inversion and time-reversal symmetry, e.g., graphene.

Saddlepoint is $T$-invariant

$$\cos\left(\frac{\Omega_1 + \Omega_2}{2} + \text{phase}(\mathcal{T})\right) = |\mathcal{T}|$$

Two dHvA harmonics with intercepts $\gamma_\pm = \varphi_B + \pi + \text{phase}(\mathcal{T}) - \cos^{-1}|\mathcal{T}|$

Two independent, identical orbits

$|\mathcal{T}| = 1$

A single orbit

$1/\sqrt{2}$
For both metals, \( \gamma_{\pm}(\mu) \) covers a \( \pi \)-interval owing to the Lifshitz transition.

A topological invariant that nonperturbatively encodes tunneling:

\[
\gamma_{\pm} = \phi_B + \pi + \text{phase}(\mathcal{T}) - \cos^{-1}|\mathcal{T}|
\]

Analogy with topological insulators: as a function of crystal momentum, the Berry phase covers a \( 2\pi \)-interval or a rational fraction of a \( 2\pi \)-interval

(Fu, Kane; Soluyanov, Vanderbilt; Rui Yu et al; AA, X. Dai, Bernevig; AA, Z. Wang, Bernevig)

(AA, Bernevig, prb 93,205104; J. Hoeller, AA)
Unavoidable *intraband* breakdown in surface states of topological crystalline insulators.

SnTe

(Hsieh, Liang Fu, Nat. Comm 3:982; Serbyn, Fu, PRB 90, 035402)

Unavoidable *interband* breakdown in over-tilted Dirac fermion

(O’Brien, Diez, Beenakker, PRL 116, 236401)

\[
0 = \cos(\Omega_1 + 2\phi) + |R|^2 \cos(\Omega_1 - \Omega_2) - |T|^2
\]

\[
\rho^2 = \text{Landau-Zener tunneling probability} = 1 \text{ at Dirac point}
\]

\[
\cos\left(\frac{\Omega_1 - \Omega_2}{2}\right) = \sqrt{1 - \rho^2} \cos\left(\frac{\Omega_1 + \Omega_2}{2} + \omega\right)
\]
Analytic method to calculate magnetic energy spectrum without large-scale numerical diagonalization

Test of generalized quantization rule with O’Brien tight-binding model of over-tilted Dirac fermion.

(Phys. Rev. Lett. 116, 236401)
Take-home

Fermiology: mapping the Fermi surface from the dHvA period.

Topo-fermiology: extracting robust information about Fermi-surface wavefunction from the dHvA intercept.

\[ \gamma = \text{Maslov} + \text{Orbital moment} + \text{Berry} + \text{Zeeman} \]

For some solids, and for some field orientations, \( \gamma/\pi \) is rational. Complete symmetry analysis of \( \gamma \) (10 classes of symmetric orbits)

In the presence of breakdown, generalized Bohr-Sommerfeld quantization conditions that encode the Berry phase and the orbital moment.

When symmetry imposes commensurability,

\[ \gamma = \text{Maslov} + \text{Berry} + \text{Tunneling phase} \]