Four-dimensional semimetals with tensor monopoles: from surface states to topological responses

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Y.-Q. Zhu, N. Goldman and G.P., arXiv:2007.00549 G. P. and N. Goldman, Phys. Rev. B 99, 045154 (2019) G. P. and N. Goldman, Phys. Rev. Lett. 121, 170401 (2018)

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- Gauge theories and Abelian monopoles
- Dirac monopoles in 3D Weyl semimetals
- Tensor Berry connections
- Tensor monopoles in 4D topological semimetals

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- 3D boundary states
- Parity magnetic effect

- States of matter beyond Landau's theory
- ► Topological quantum numbers: Z, Z₂, etc.

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- Bulk-edge correspondence
- Effective Dirac Hamiltonians
- Berry connections and curvatures

U(1) gauge theories

$$\blacktriangleright L = \frac{1}{4} F_{\mu\nu} F^{\mu\nu} + A_{\mu} J^{\mu}$$

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

- $\blacktriangleright A_{\mu} \to A_{\mu} \partial_{\mu} \lambda$
- $\triangleright \ E_i = F_{i0}, \ \tilde{B}_i = \epsilon_{ijk} F^{jk}$
- $\blacktriangleright \ \partial^i \tilde{B}_i = 0$
- Dirac monopoles violate the magnetic Gauss law

•
$$L = \frac{1}{4} \mathcal{H}_{\mu\nu\lambda} \mathcal{H}^{\mu\nu\lambda} + B_{\mu\nu} J^{\mu\nu}$$

$$\blacktriangleright \mathcal{H}_{\mu\nu\lambda} = \partial_{\mu}B_{\nu\lambda} + \partial_{\nu}B_{\lambda\mu} + \partial_{\lambda}B_{\mu\nu}$$

$$\blacktriangleright B_{\mu\nu} \to B_{\mu\nu} + \partial_{\mu}\xi_{\nu} - \partial_{\nu}\xi_{\mu}$$

•
$$\tilde{E}_{ij} = \mathcal{H}_{ij0}, \ \tilde{B}_i = \epsilon_{ijkl} \mathcal{H}^{jkl}$$

$$\blacktriangleright \ \partial^i \tilde{B}_i = 0$$

 Tensor monopoles violate the magnetic Gauss law

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Monopoles and topological invariants

Monopoles allow us to prove the quantization of the electric charge.



The first and second **Chern numbers** characterize monopoles in 3D (Dirac monopole) and 5D (Yang monopole), respectively.

Tensor monopoles in 4D are characterized by the **Dixmier-Douady** (\mathcal{DD}) invariant (Murray, 1996).

3D Dirac monopoles

U(1) vector gauge field: $A_{\mu} \rightarrow A_{\mu} - \partial_{\mu}\lambda$.

Curvature tensor: $F_{\mu\nu} = \partial_{\mu}A_{\nu} - \partial_{\nu}A_{\mu}$.

$$ilde{B}^{j} = rac{r^{j}}{|r|^{3}},$$

 $r^{j} = \{x, y, z\}, \quad r = \sqrt{x^{2} + y^{2} + z^{2}}.$

First Chern number:

$$Q = \frac{1}{2\pi} \int_{S^2} dx^k \wedge dx^l F_{kl} = \pm \frac{1}{2\pi} \int_0^\pi d\theta \int_0^{2\pi} d\phi \sin \theta = \pm 1.$$

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4D tensor monopoles

U(1) tensor gauge field: $B_{\mu\nu} \rightarrow B_{\mu\nu} + \partial_{\mu}\xi_{\nu} - \partial_{\nu}\xi_{\mu}$. Curvature tensor: $\mathcal{H}_{\mu\nu\lambda} = \partial_{\mu}B_{\nu\lambda} + \partial_{\nu}B_{\lambda\mu} + \partial_{\lambda}B_{\mu\nu}$.

$$ilde{B}^{j} = rac{r^{j}}{|r|^{4}},$$

 $r^{j} = \{x, y, z, w\}, \quad r = \sqrt{x^{2} + y^{2} + z^{2} + w^{2}}.$

First DD number:

$$Q_{\mathcal{T}} = \frac{1}{2\pi^2} \int_{S^3} dx^k \wedge dx^l \wedge dx^m \mathcal{H}_{klm} = \pm \frac{1}{2\pi^2} \int_0^{\pi} d\theta_1 \int_0^{\pi} d\theta_2 \int_0^{2\pi} d\varphi \sin^2 \theta_1 \sin \theta_2 = \pm 1.$$

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Berry connection

Bloch wavefunctions: $|u(\mathbf{q})\rangle = (u^1(\mathbf{q}), u^2(\mathbf{q}), ..., u^{\aleph}(\mathbf{q}))^{\top}$.

The gauge redundancy in a non-degenerate Bloch state is encoded in the arbitrary phase in $|u\rangle$

$$|u\rangle
ightarrow e^{i\alpha(\mathbf{q})}|u
angle,$$

where $\alpha(\mathbf{q})$ is a momentum-dependent function. We can build an Abelian gauge connection in momentum space:

$$A_j = i \langle u | \partial_j | u \rangle, \quad A_j \to A_j - \partial_j \alpha$$

with $\partial_j \equiv \partial_{q_i}$, while the gauge-invariant Berry curvature is given by

$$\Omega_{jk}=\partial_j A_k-\partial_k A_j.$$

3D Weyl semimetals





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$$H_{\rm 3D} = q_x \sigma^x + q_y \sigma^y + q_z \sigma^z,$$

where $\boldsymbol{q} = (q_x, q_y, q_z)$ are the momenta and $\sigma^{x,y,z}$ are the Pauli matrices.

In 3D Weyl semimetals, the Berry curvature of the Dirac monopole is given by

$$\Omega_{jk} = \epsilon_{jkl} \frac{q_l}{2(q_x^2 + q_y^2 + q_z^2)^{3/2}},$$

$$Q=rac{1}{2\pi}\int_{S^2} dq^j\wedge dq^k\Omega_{jk}=\pm 1.$$

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Tensor Berry connection

$$B_{jk} = \frac{i}{3} \, \epsilon^{abc} \phi_a \partial_j \phi_b \partial_k \phi_c,$$

where $a, b, c = \{1, 2, 3\}.$

Scalars can be complex or (pseudo-)real depending on their gauge transformations

$$\begin{split} \phi &\to e^{i\alpha(\mathbf{q})}\phi, \\ \varphi &\to \varphi + \alpha(\mathbf{q}). \end{split}$$

In our case, we consider the following scalars

$$\phi_1 \equiv \varphi \rightarrow \varphi + \alpha(\mathbf{q}), \quad \phi_2 \rightarrow e^{-i\alpha(\mathbf{q})}\phi_2, \quad \phi_3 \rightarrow e^{i\alpha(\mathbf{q})}\phi_3,$$

such that

$$B_{jk} \to B_{jk} + \Lambda_{jk},$$

$$\mathcal{H}_{jkl} = \partial_j B_{kl} + \partial_k B_{lj} + \partial_l B_{jk}.$$

$$H(\mathbf{k}) = d_{x}\tilde{\Gamma}_{x} + d_{y}\tilde{\Gamma}_{y} + d_{z}\tilde{\Gamma}_{z} + d_{w}\tilde{\Gamma}_{w}, \qquad (1)$$

with the four-component Bloch vector defined as

$$d_{x} = 2J \sin k_{x}, \ d_{y} = 2J \sin k_{y}, \ d_{z} = 2J \sin k_{z}, d_{w} = 2J(M - \cos k_{x} - \cos k_{y} - \cos k_{z} - \cos k_{w}).$$
(2)

with

$$\begin{split} \tilde{\Gamma}_{x} &= \sigma_{0} \otimes \sigma_{1} + a \, \sigma_{1} \otimes \sigma_{0}, \quad \tilde{\Gamma}_{y} = \sigma_{2} \otimes \sigma_{3} + a \, \sigma_{3} \otimes \sigma_{2}, \\ \tilde{\Gamma}_{z} &= \sigma_{0} \otimes \sigma_{2} + a \, \sigma_{2} \otimes \sigma_{0}, \quad \tilde{\Gamma}_{w} = \sigma_{1} \otimes \sigma_{3} + a \, \sigma_{3} \otimes \sigma_{1}. \end{split}$$

These matrices only satisfy the Clifford algebra for a = 0 ("Dirac regime"). When $a \neq 0$, the Hamiltonian (1) supports spin-3/2-like quasiparticles (birefringent fermions).

Monopole-to-monopole phase transition

For a = 0 we have a Z_2 monopole protected by CP symmetry.



$$E(\mathbf{k}) = \pm (1 \pm a) \sqrt{d_x^2 + d_y^2 + d_z^2 + d_w^2}.$$
 (3)

For 2 < M < 4 and $a \neq 0$, there exists a single pair of Dirac-like cones in the first Brillouin zone (BZ) separated along the k_w axis and located at $\mathbf{K}_{\pm} = (0, 0, 0, \pm \arccos k_m)$ with $k_m = M - 3$.

$$\mathcal{DD} = \frac{1}{2\pi^2} \int_{\mathbb{S}^3} dq^j \wedge dq^k \wedge dq^l \sum_{n=1,2} \mathcal{H}^n_{jkl}, \qquad (4)$$

where

$$\mathcal{H}_{jkl}^{n} = \partial_{j} B_{kl}^{n} + \partial_{k} B_{lj}^{n} + \partial_{l} B_{jk}^{n}, \qquad (5)$$

denotes the 3-form Berry curvature associated with the *n*-th eigenstate $|u_n(\mathbf{q})\rangle$. Only the two lowest bands (n=1,2) contribute to the \mathcal{DD} invariant, as required by the half-filling condition.

$$B_{jk}^n = \phi_n \mathcal{F}_{jk}^n, \ \phi_n = -\frac{i}{2} \log \prod_{\aleph=1}^4 u_{-,n}^\aleph, \tag{6}$$

where u_n^{\aleph} denotes the components of $|u_n\rangle$.

3D boundary states



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Parity magnetic effect and topological currents

we introduce the dipolar momentum b_{μ} , which denotes the separation of the two monopoles in momentum space, with vector $\boldsymbol{b} = (\boldsymbol{K}_{+} - \boldsymbol{K}_{-})/2$, and in energy with offset $2b_t$.

$$H_{\rm eff} = k_i \tilde{G}^i - b_\mu \tilde{G}^\mu_b, \tag{7}$$

where i = x, y, z, w and $\mu = t, x, y, z, w$.

By implementing a Legendre transformation on Eq. (7), the action can be written in terms of a first-order Lagrangian,

$$S[\bar{\psi},\psi,b] = \int d^5 x \,\bar{\psi} (i\tilde{\gamma}^{\mu}\partial_{\mu} - \tilde{\gamma}^{\mu}_{b}b_{\mu})\psi.$$
(8)

By integrating out the fermion field, we obtain the effective action

$$S_{\rm eff} = -i \ln \det(i \tilde{\gamma}^{\mu} D_{\mu} - \tilde{\gamma}^{\mu}_{b} b_{\mu}), \qquad (9)$$

where $D_{\mu} = \partial_{\mu} - iA_{\mu}$ is the gauge covariant derivative.

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Parity anomaly

This action can be regularized by employing the standard Pauli-Villars method which consists in introducing a mass term $\tilde{m}\bar{\psi}\psi$ with $\tilde{m} = m - \alpha k^2$.

We determine the effective Chern-Simons action, by calculating a one-loop triangle diagram

$$S_{\rm top} = \frac{C_2}{4\pi^2} \int d^5 x \, \epsilon^{\mu\nu\lambda\rho\sigma} b_\mu \partial_\nu A_\lambda \partial_\rho A_\sigma, \qquad (10)$$

where $C_2 = -[\operatorname{sgn}(m) + \operatorname{sgn}(\alpha)]/2$ is the second Chern number.

Our massless Hamiltonian in the Dirac case, supports a reflection symmetry along the w direction, namely

$$U_r^{-1}H(k_x, k_y, k_z, k_w)U_r = H(k_x, k_y, k_z, -k_w),$$
(11)

with $U_r = \sigma_2 \otimes \sigma_0$, which is broken at quantum level by the Pauli-Villars mass regulator. This is the essence of the parity anomaly for a = 0 (similar situation with the spin-3/2-like fermions and the sublattice chiral symmetry).

Topological current

$$J^{\mu} = \frac{\delta S_{\text{top}}}{\delta A_{\mu}} = \frac{C_2}{2\pi^2} \epsilon^{\mu\nu\lambda\rho\sigma} \partial_{\nu} b_{\lambda} \partial_{\rho} A_{\sigma}.$$
 (12)

For simplicity, we consider the response of our system to a static and uniform magnetic field (i.e. $A_y = xB^z$ and $A_{x,z,w,t} = 0$), and to a simultaneous time-dependent modulation of the cones separation, $b_w = \arccos[M(t) - 3]$:

$$J^{z} = \frac{C_2}{2\pi^2} (\partial_t b_w) B^z.$$
(13)

This is the parity magnetic effect, where b_w plays the role of an effective axial gauge field.



▶ 4D topological semimetals protected by chiral symmetry.

- Monopole-to-monopole phase transition $(Z_2 \rightarrow Z)$.
- Robust 3D edge states.
- 4D parity magnetic effect.

Experimental Observation of Tensor Monopoles

The three-level model proposed in "G.P. and N. Goldman, PRL (2018)" has been recently implemented in superconducting qudits:

Experimental Observation of Tensor Monopoles with a Superconducting Qudit

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ArXiv:2006.11770.

They have measured the DD invariant from the quantum metric following "G.P. and N. Goldman, PRL (2018)".