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The Chiral Anomaly Factory: Creating Weyls with a Magnetic Field

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Weyl fermions can be created in materials with both time reversal and inversion symmetry by applying a magnetic field, as evidenced by recent measurements of anomalous negative magnetoresistance. Here, we do a thorough analysis of the Weyl points in these materials: by enforcing crystal symmetries, we classify the location and monopole charges of Weyl points created by fields aligned with high-symmetry axes. The analysis applies generally to materials with band inversion in the T_d , D_{4h} and D_{6h} point groups. For the T_d point group, we find that Weyl nodes persist for all directions of the magnetic field. Further, we compute the anomalous magnetoresistance of field-created Weyl fermions in the semiclassical regime. We find that the magnetoresistance can scale non-quadratically with magnetic field, in contrast to materials with intrinsic Weyl nodes. Our results are relevant to future experiments in the semi-classical regime.

INTRODUCTION

Following their insulating counterparts[1], topological semi-metals have attracted much recent theoretical and experimental interest. Weyl and Dirac semimetals have recently been theoretically predicted [2–6] and experimentally observed [7–9]. Both display topologically protected Fermi-arc surface states, as well as large negative magnetoresistance due to the "chiral anomaly" [10–15]. While Weyl fermions in these semimetals are robust to small perturbations due to their topological character, Dirac points require a combination of crystal symmetry, time reversal, and inversion symmetry [16]. This suggests that Weyl fermions can be engineered by breaking inversion or time reversal symmetry in materials with four-band crossings. While breaking inversion symmetry can be accomplished by adding strain[17], it is more straightforward to break time reversal symmetry by turning on a magnetic field. This route to creating Weyl fermions has already been carried out in GdPtBi[18, 19], NdPtBi[19], $Na_3Bi[13]$ and $Cd_3As_2[20-22]$. We predict that the same route can be used to observe Weyl fermions in the experimentally relevant materials HgTe[23, 24] and InSb[25].

Here, we consider turning on a magnetic field in materials with four-band crossings. We consider two types of four-band crossings: symmetry-enforced band crossings at the Γ point and Dirac points near the Γ point on a high-symmetry line. In both cases, the magnetic field breaks the four-band crossing into an even number of Weyl nodes. We demonstrate the emergence of Weyl nodes explicitly in GdPtBi, HgTe and InSb, which host a symmetry-enforced four-band crossing near the Fermi level, and Cd₃As₂ and Na₃Bi, which host Dirac points near the Fermi level, using $k \cdot p$ Hamiltonians generated by ab initio calculations. We then show that this is a general result when the magnetic field is along a high-symmetry line. However, the emergent Weyls do not always reside on the axis parallel to the magnetic field: instead, a complex map of Weyl points (and nodal lines [26–29]) emerges for different directions of the magnetic field. Since Weyl points do not require symmetry protection, they persist when the magnetic field is moved away from these axes. Surprisingly, we find that in GdPtBi and HgTe, Weyl points exist for all directions of the magnetic field. In the Supplement, we give numerical evidence for this statement and then prove it explicitly for all materials with T_d symmetry and j = 3/2 orbitals at the Fermi level.

We emphasize that while we use the language of applying an external magnetic field, our results apply equally well to magnetically ordered materials that host a fourband crossing above the Néel temperature and can thus be tuned to display Weyl points below this temperature. This is relevant for antiferromagnetic Heuslers[19].

Finally we consider the semiclassical negative magnetoconductance that is a consequence of the chiral anomaly. This has previously been considered for Weyl points that exist independent of the magnetic field[30, 31]. Here, we show that when the Weyl points are created by a magnetic field, the magnetoconductance takes a different scaling form. In particular, it can scale as high as $B^{5/2}$, where the exact scaling depends on the linearized Hamiltonian near the Weyl point. We apply this model to GdPtBi, in which recent experiments[18] have observed the chiral anomaly.

EMERGENT WEYL NODES FROM A SYMMETRY-ENFORCED FOUR-BAND CROSSING

Here we focus on GdPtBi, which is in the T_d point group. However, because our analysis depends only on symmetry and band inversion, it applies to all materials with the same symmetry and relevant orbitals near the Γ point, e.g., HgTe and InSb.

In GdPtBi, the low-energy spectrum near the Γ point is described by the four *p*-orbitals with $j_z = \pm 3/2, \pm 1/2$. Thus, the symmetry operators comprise

a four-dimensional representation of the T_d symmetry group. The $k \cdot p$ Hamiltonian takes the form[32],

$$H_{\Gamma}(k_x, k_y, k_z) = \left(A_0 + (A + \frac{C}{\sqrt{3}})k^2\right)I_{4\times4} + C(k_x^2 - k_y^2)\Gamma_1 + \frac{C}{\sqrt{3}}(2k_z^2 - k_x^2 - k_y^2)\Gamma_2 + E(k_xk_y\Gamma_3 + k_xk_z\Gamma_4 + k_yk_z\Gamma_5) + D(k_xU_1 + k_yU_2 + 2k_zU_3),$$
(1)

where the $\Gamma_{1,...,5}$ are Clifford algebra matrices, $\Gamma_{ij} = [\Gamma_i, \Gamma_j]/(2i)$ and $U_1 = \sqrt{3}\Gamma_{15} - \Gamma_{25}, U_2 = -\sqrt{3}\Gamma_{14} - \Gamma_{24}, U_3 = \Gamma_{23}$. The parameters A_0, A, C, D, E are obtained by an ab initio fit and given in the Supplementary Material. We note here only that $A_0 \approx 0$, meaning that at the Fermi level the spectrum is four-fold degenerate at the Γ point[18]; two bands disperse upwards and two disperse downwards. The $D \neq 0$ parameter breaks inversion symmetry.

We now consider what happens in the presence of a magnetic field by adding an effective Zeeman coupling to Eq (1),

$$H_Z = \vec{B} \cdot \vec{J},\tag{2}$$

where \vec{J} is a vector of the spin-3/2 matrices. Using this model, oppositely-dispersing bands have either a protected or avoided crossing, *regardless* of their *g*-factor. Notice that band inversion is crucial here: if all bands dispersed in the same direction, then the presence or absence of a crossing would depend crucially on the precise values *g*-factors of the bands. However, as long as the system exhibits band inversion, and all bands have the same sign of the *g*-factor, then the physics described below is universal. In the following analysis, we will ignore the effects of cyclotron motion to lowest order, focusing purely on the Zeeman splitting. This is a good approximation for large *g*-factor materials such as GdPtBi.

When the magnetic field is along an axis of rotation, band crossings along this axis between bands with different eigenvalues under the rotation are protected; thus, Weyl points are guaranteed to exist. Because the original four-band quadratic crossing was at the Fermi energy at zero field, these Weyl points will also lie near the Fermi level. Additionally, since the nontrivial Chern number of a Weyl point cannot disappear under small deformations of the Hamiltonian, these Weyls will continue to exist even as the magnetic field is moved away from the rotation axis. This protection is crucial to experimental observation. However, as the magnetic field is moved far away from a high-symmetry axis, it is possible for two Weyl points of opposite chirality to meet and annihilate. Surprisingly, we have verified numerically, using the $k \cdot p$ Hamiltonian (1), that this is not the case for every pair of nodes: Weyl points exist in GdPtBi for all directions of the magnetic field.

Weyl points can also be protected between highsymmetry planes with different Chern numbers; we

\vec{B}	Emergent Weyl points
[001], [010], [100]	$6 + 8k_1$ Weyl points
$[110], [1\overline{1}0], [101],$	0, 1, or $2 $ line nodes,
$[10\bar{1}], [011], [01\bar{1}]$	$4 + 8k_2$ Weyl points
[111],	
$[11\bar{1}], [1\bar{1}1], [\bar{1}11],$	$4 + 6k_3$ Weyl points
$[\bar{1}\bar{1}1], [\bar{1}\bar{1}1], [1\bar{1}\bar{1}]$	

TABLE I. Weyl points in GdPtBi when a magnetic field is applied along one of the high-symmetry axes in the first column. The integers k_i indicate Weyl points that appear at generic points Brillouin zone; for GdPtBi, a numerical analysis of our $k \cdot p$ model yields $k_1 = k_2 = 0, k_3 = 1$, but these numbers are material-dependent.

show[32]that in GdPtBi, when the magnetic field is applied along the \hat{z} direction, two such Weyl points exist in the $k_x = 0$ plane and another pair in the $k_y = 0$ plane. These points persist –albeit moving in momentum-space–when the magnetic field is moved off this axis until they reach each other and annihilate. The same analysis applies to a magnetic field in the \hat{x} and \hat{y} directions.

When the magnetic field is in the $\hat{x} + \hat{y}$ direction, we find four Weyl nodes which, for $D \to 0$, are confined to the (k, k, k_z) plane; these nodes persist as D is continuously varied from zero to its experimentally relevant value in either GdPtBi or HgTe. Additionally, at least one line node appears in the $(k, -k, k_z)$ plane.[32]For the ab initio parameters, two line nodes appear; however, for other choices of parameters, one of these lines moves towards the edge of the Brillouin zone and disappears.

Last, when the magnetic field is in the $\hat{x} + \hat{y} + \hat{z}$ direction, there are four Weyl points along the $k_x = k_y = k_z$ axis.

Additional Weyl points at generic points in the Brillouin zone must occur in multiples of six or eight, depending on the symmetry that remains when a particular magnetic field is present. A summary of Weyl points that emerge in GdPtBi upon applying a magnetic field along a high-symmetry axis are shown in Table I.

The symmetry-protected Weyl points we describe in this section also persist for arbitrary magnetic fields. In particular, at the special point E = 2C, D = 0 in Eq (1), the Hamiltonian $H_{\Gamma} + H_Z$ is exactly solvable and has Weyl points along the momentum axis parallel to the magnetic field. We show in the Supplement that as E is moved away from this fine-tuned value, the Weyl points move in space, but do not annihilate; we confirm this claim with a numerical analysis. Because the Weyl points are topologically protected, they will also persist for small values of D.

EMERGENT WEYL NODES FROM DIRAC POINTS NEAR THE Γ POINT

In Cd₃As₂ and Na₃Bi, a different, but similar, scenario develops, where again band inversion plays a crucial role. There are two pairs of relevant orbitals at the Γ point near the Fermi level: the *s*-orbitals with $j_z = \pm 1/2$ and the *p*-orbitals with $j_z = \pm 3/2$; each pair transforms as a two-dimensional representation of D_{nh} , where n = 4in Cd₃As₂ and n = 6 in Na₃Bi. The two representations have different energies at the Γ point, but, because the bands are inverted, they can cross elsewhere in momentum space. In the materials of interest, the crossings occurs at the Fermi level and are protected by C_{nz} symmetry. Furthermore, the crossings occur close enough to the Γ point to be described by the effective $k \cdot p$ model,

$$H_{\text{Dirac}}(k_x, k_y, k_z) = \left(C_0 + C_1 k_z^2 + C_2 k_{\parallel}^2\right) I_{4 \times 4} + (3)$$

$$\tau_z \otimes \left(\left(M_0 + M_1 k_z^2 + M_2 k_{\parallel}^2\right) \sigma_z + A(\sigma_x k_x + \sigma_y k_y)\right),$$

where $k_{\parallel}^2 = k_x^2 + k_y^2$. Eq (3) describes two Dirac points on the k_z axis at $k_z = \pm \sqrt{-M_0/M_1}$ (M_0 and M_1 have opposite signs in the ab initio fit; the fitting parameters for the quadratic terms and the symmetry-allowed third order terms are included in the Supplementary Material.) Because the four relevant bands come in pairs with distinct angular momentum character, we allow for two different g-factors g_s and g_p in the Zeeman coupling [32]. In the presence of a magnetic field, each Dirac point can split into up to four Weyl points. As in the previous section, putative crossings will exist regardless of the qfactors of the different orbitals because the bands disperse in opposite directions. Furthermore, Weyl points that emerge when the magnetic field is along a particular high-symmetry axis must persist when the field is slightly off-axis because they can only annihilate in pairs of opposite chirality.

We now summarize our results[32]. When the magnetic field is along the \hat{z} direction all band crossings are protected by C_{nz} symmetry: depending on the value of the magnetic field, this implies between four and eight Weyl points. Band crossings between the $j_z = \pm 3/2$ and $\pm 1/2$ bands are double Weyl points – these are not robust to small changes in the magnetic field; instead, they can split into two single Weyl points. Line nodes, protected by M_{001} , can also emerge in the $k_z = 0$ plane for large enough magnetic field.

When the magnetic field is along the \hat{x} direction, C_{2x} symmetry can protect between two and four total Weyl points and M_{100} symmetry protects line nodes in the $k_x = 0$ plane. The same is true for the other symmetry-related directions.

SEMICLASSICAL MAGNETOTRANSPORT

The presence of Weyl points near the Fermi surface in a material - whether intrinsic or created by an external field - leads to an experimentally measurable negative magnetoresistance.[13–15, 18] The origin of this effect is due to the non-trivial Berry curvature surrounding each Weyl node, and is a manifestation of the so-called "chiral anomaly." Previous theoretical analysis of this effect has been carried out for materials with intrinsic, field independent Weyl nodes, in both the semiclassical and ultra-quantum (only the lowest Landau level occupied) limits.[12, 30, 31, 33] For these intrinsic Weyls, chiral kinetic theory implies that, in the semiclassical limit and at low temperature, there is an anomalous positive magnetoconductance of the form

$$\sigma_a^{\mu\nu} = \sum_i \frac{\tau v_i^3}{8\pi^2 \mu_i^2} B^\mu B^\nu,$$

where τ is the inter-nodal scattering rate, v_i is the (geometric) mean velocity of node *i*, and μ_i is the chemical potential measured from node *i*. We wish to generalize this result to the case where the Weyl nodes are created by an external magnetic field. Relegating the details of the derivation to the Supplementary material, we find that the magnetoconductance acquires additional field dependence due to the field dependence of the Weyl velocities, which enters both explicitly and through the now-strongly-field-dependent scattering time. We find for low fields

$$\sigma_a^{\mu\nu} = \sum_i \frac{\tau^i(B) |\det A^i|}{8\pi^2 \mu_i^2} B^{\mu} B^{\nu} (1 + \mathcal{O}(B)).$$
(4)

where A^i , along with the vector u^i , which, in the materials we consider, enters the $\mathcal{O}(B)$ corrections, parameterize the linearized two-band Hamiltonian near the Weyl point at k^i :[34]

$$H = u_j^i (k_j - k_j^i) \mathbb{I} + (k_j - k_j^i) A_{jk}^i \sigma_k$$
(5)

 $\tau^i(B)$ is the rate for scattering out of node i. For short-range impurities we find

$$\tau^{i}(B) = \tau_{0} \frac{2\pi^{2} |\det A^{i}|}{\mu_{i}^{2}} (1 + \mathcal{O}(B))$$
(6)

We now make three observations. First, because $|\det A^i|$ depends on magnetic field, we expect that the magnetoconductance for field-created Weyls scales differently than that for intrinsic Weyl semimetals; in particular, we provide a simple model in the Supplementary Material where $|\det A^i| \sim |B|^{1/2}$. Second, because $|\det A^i|$ is not a rotationally invariant function of **B**, we expect that the magnetoconductance will also fail to be rotationally invariant. Finally, as **B** increases, we expect

the $\mathcal{O}(B)$ corrections to Eq. (4), given explicitly in the Supplementary material, to become significant. This can cause the directionality of the magnetoconductance to acquire additional field-dependence.

Similarly, thermoelectric transport in Weyl materials is also influenced by the chiral anomaly. In particular, the thermoelectric conductivity $\alpha^{\mu\nu}$, relating the current response to a temperature gradient, is experimentally relevant. Using Onsager reciprocity[35, 36], we can compute this by looking instead at the energy current response to an electric field. Using the same semiclassical treatement as above and neglecting interactions we recover the Mott formula

$$\alpha^{\mu\nu} = \frac{\pi^2 T^2}{3} \frac{\partial \sigma^{\mu\nu}}{\partial \mu},\tag{7}$$

valid for both the anomalous and non-anomalous parts of the thermoelectric conductivity. In particular, we expect that the magnetic field dependence of the anomalous thermoelectric conductivity should simply follow that of the ordinary conductivity. Differences between these two effects serves to measure the significance of electronelectron interactions, which explicitly modify the heatcurrent[37].

Lastly, we remark on the effects of higher-order Weyl crossings on magnetotransport. In particular, we focus on double-Weyl points, since – as mentioned above – these are present in Na₃Bi and Cd₃As₂. Using the fact that the Berry curvature transforms as a tensor under reparametrizations of the Brillouin zone, we can easily repeat the semiclassical analysis above for double (or even *n*-fold) Weyl points. We find that the forms of all transport coefficients remain the same. The only change is that the response coefficients are proportional to the square of the Chern number (i.e. 4 in the case of a double Weyl), and that the form of the density of states changes. In particular, the density of states for a double Weyl point is linear in the chemical potential.

VALIDITY OF SEMICLASSICAL TRANSPORT

We now consider whether Weyl points can be well separated when the system is in the semiclassical regime. This introduces two competing criteria. First, the Weyl points must be well-resolved: the Fermi level must be close enough to the nodal point that the Fermi surface consists of disconnected pockets encircling each node. Quantitatively, this translates to the constraint,

$$k_F \sim \frac{\mu}{v} \ll k^0 \tag{8}$$

where $v = (\det A)^{1/3}$ is the mean velocity of the Weyl point at position k^0 , k_F is the Fermi wavevector measured as the deviation from k^0 , and the chemical potential μ is the deviation in energy from the Weyl point. Second, we demand that the number ν of filled Landau levels is large. Recall that for a single Weyl point,

$$\mu \sim \sqrt{2B\nu}.\tag{9}$$

Hence, we demand,

$$\mu \gg \sqrt{2B} \tag{10}$$

We now consider when the two constraints (8) and (10) are simultaneously satisfiable. For Weyl points that originate from a symmetry-enforced band touching, such as those in GdPtBi, $v \sim k^0 \sim \sqrt{B}$, and hence we need simultaneously that

$$B \gg \gamma_1 \mu$$
 and $B \ll \gamma_2 \mu^2$ (11)

where γ_1 and γ_2 are material-dependent parameters. Whether or not there exists a regime that satisfies Eq (11)depends on μ , which is nearly fixed (for B not too large) for a bulk 3d material. For GdPtBi, we find from experiment [18] that the Weyl points become well resolved for $B \sim 6T$; however quantum oscillations reveal that the Landau level index $\nu \sim 5$ at this value of the field. However, the preceding analysis ignores the magnetization of GdPtBi. Near the Néel temperature of about 9K, the spins will have a large magnetic susceptibility, in which case a smaller field will have the same effect. Additionally, this will be compounded by the quenching of the orbital magnetism in the crystal, leading to an enhancement of the Zeeman energy relative to the cyclotron energy. In this case, it is quite possible that the experimental regime satisfies Eq (11)[19].

If the scale of inversion breaking, D in Eq (1), is much larger than the magnetic field, then $k^0 \sim \sqrt{B}$ and $v \sim D$. Then Eq (11) is replaced by,

$$\gamma_1 \mu \ll D\sqrt{B} \text{ and } \sqrt{B} \ll \gamma_2 \mu,$$
 (12)

which is satisfied for small enough fields when D exceeds other scales.

We now consider Weyl points that emerge from splitting a Dirac point with a magnetic field. In this case, for the two Weyl points to be well-resolved, the spacing between the Weyl points, which scales like B, must be greater than $k_F \sim \mu/v$. To leading order, v depends on the initial dispersion (i.e., determined by Eq (3)) and only has sub-leading B dependence. This again leads to Eq (11). The recent experiment on Na₃Bi[13] reports the nodes to be well separated when B = 12T, but the onset of the lowest Landau level to be near 6 - 8T. Hence, the semiclassical regime will likely not quantitatively describe this experiment.

DISCUSSION

A magnetic field can create Weyl points from fourband crossings by breaking time reversal symmetry. This is a powerful technique for creating Weyl points whose position in energy-momentum space is tunable. Here, we have studied two canonical and experimentally relevant examples: a symmetry-enforced four-band crossing at the Γ point and a Dirac node near the Γ point. We have shown that a complex map of Weyl points (and line nodes) emerges, depending on the direction and magnitude of the magnetic field. It would be interesting to experimentally track the movement of these points by observing how the surface Fermi arcs move as the magnetic field is changed, e.g., in STM experiments. Furthermore, for the particular cases of GdPtBi and HgTe, our numerical analysis indicates that Weyl points exist near the Fermi level for all directions of the magnetic field: this should prompt future experiments that probe the chiral anomaly with fields away from the high-symmetry axes.

We computed the anomalous longitudinal conductance in the semiclassical regime for Weyl points created by a magnetic field. The conductance scales with a higher power of the magnetic field than the conductance for intrinsic Weyl points. Naively, this is consistent with experimental data: for example, the low-field data in Ref 18 shows that σ_{xx} scales like a higher power of B than B^2 ; we plot this data in the Supplement. However, this agreement should be taken with a grain of salt, because, as mentioned in the previous section, the experiment is not fully in the semi-classical regime. Our theory will be better tested in future experiments that are in this regime, where we expect the scaling of longitudinal conductance to go beyond B^2 for magnetic-field created Weyl points.

Our analysis readily generalizes to other point groups. This would be a useful course of study to identify future candidates for magnetic field created Weyl points. In addition, an analysis of the quantum regime could be used to describe existing experiments. We leave these questions for future works.

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