

Diabological touching point in the magnetic energy levels of topological nodal-line metalsChong Wang^{1,*}, Zhongyi Zhang^{2,*}, Liqin Zhou², Hongming Weng², Chen Fang^{2,†} and A. Alexandradinata^{3,‡}¹*Department of Physics, Carnegie Mellon University, Pittsburgh, Pennsylvania 15213, USA*²*Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China*³*Department of Physics and Institute for Condensed Matter Theory, University of Illinois at Urbana-Champaign, Urbana, Illinois 61801, USA*

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For three-dimensional metals, Landau levels disperse as a function of the magnetic field and the momentum wave number parallel to the field. In this two-dimensional parameter space, it is shown that two conically dispersing Landau levels can touch at a diabological point—a *Landau-Dirac point*. The conditions giving rise to Landau-Dirac points are shown to be magnetic breakdown (field-driven quantum tunneling) and certain crystallographic spacetime symmetry. Both conditions are realizable in topological nodal-line metals, as we exemplify with the material candidates CaX_3 ($X = \text{As}, \text{P}$). The experimental fingerprints of a Landau-Dirac point include (a) anomalous “batman”-like peaks in the magnetoresistance, (b) circular Landau-Fermi surfaces revealed by angle-dependent ultrasonic attenuation, and (c) the tunability of the frequency onset of optical absorption to zero.

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For a real Hamiltonian, energy-level surfaces over a two-dimensional parameter space can locally form a double cone (*diabolo*) with an energy-degenerate vertex known as a *diabological point* [1–4]. The first physical application of the diabological point was by Hamilton in his 1832 prediction of conical refraction [5,6]. Since then, the diabological point has re-emerged in diverse phenomena in singular optics [7], chemistry [8–10], and nuclear [11] and quantum [12] physics. Its most recent revival is as Dirac-Weyl points [13] in the crystal-momentum space of topological semimetals [14–18] and insulators [19–22].

This work presents another type of diabological point in a textbook solid-state phenomenon: the quantized energy spectrum of three-dimensional metals subject to a homogeneous magnetic field. A fundamental feature of the magnetic energy spectrum is its quantization into Landau levels [23], which are naturally parametrized by the field magnitude (B) and the momentum wave number (k_z) parallel to the field. In this two-dimensional parameter space, Fig. 1(b) illustrates how two Landau-level surfaces can touch at a diabological point, which will be referred to as a *Landau-Dirac point*. Parallel transport around an equienergy contour of the Landau-Dirac cone gives a topologically quantized, π Berry phase [24].

Landau-Dirac points do *not* exist for metals with a single Fermi pocket; their Landau levels are determined by the Onsager-Lifshitz-Roth quantization rule [25–27]: $\hbar/eB = (2\pi n + \gamma)/S(E, k_z)$, with $S(E, k_z)$ the \mathbf{k} area enclosed by the orbit, $0 \leq n \in \mathbf{Z}$ the Landau-level index, and $\gamma \approx 1$ being field independent to leading order in B [27–30]. Henceforth,

we set $\hbar = e = 1$ so that B^{-1} equals the square of the magnetic length. Generally for an electron-like (resp. hole-like) pocket, $S(E, k_z)$ is a single-valued function of k_z and an increasing (resp. decreasing) function of energy E , e.g., $S = \pi(2mE - k_z^2)$ for a free-electron gas with mass m . These conditions on $S(E, k_z)$ ensure that equienergy solutions of the quantization rule lie on *open*, nonintersecting contours in (B^{-1}, k_z) space, as illustrated for the free-electron gas in Fig. 1(a). It follows that the *closed* equienergy contours of the diabolo [cf. Fig. 1(b)] cannot derive from a single electron-like or hole-like pocket.

However, if multiple pockets are linked by field-driven quantum tunneling (known as magnetic breakdown [31–35]), we will show that tunneling-induced level repulsion can convert open contours to closed contours of a diabolo. A stable Landau-Dirac point relies on certain crystallographic symmetries that are preserved in the presence of the field. For example, the composition Tc_{2y} of time reversal and twofold rotation (about a field-orthogonal axis) maps $(B^{-1}, k_z) \rightarrow (B^{-1}, k_z)$, ensuring that Landau-Dirac points are movable over (B^{-1}, k_z) space, but irremovable unless annihilated in pairs—as analogous to Dirac points in graphene [15]. Either spatial inversion $i [(x, y, z) \rightarrow (-x, -y, -z)]$ or reflection $\tau_z [(x, y, z) \rightarrow (x, y, -z)]$ maps $(B^{-1}, k_z) \rightarrow (B^{-1}, -k_z)$, and therefore protects crossings between Landau levels of opposite i (or τ_z) representations on high-symmetry lines. All three symmetries, plus the condition of magnetic breakdown, are realizable in topological nodal-line metals [36–41], as we will first demonstrate with a conceptually simple, minimal model, and subsequently for the nodal-line metallic candidates CaX_3 ($X = \text{As}, \text{P}$). We will show further that a Landau-Dirac point reveals itself in anomalous “batman”-like peaks in the density of states [cf. Fig. 1(b)], as well as having unique fingerprints in ultrasonic attenuation and optical absorption.

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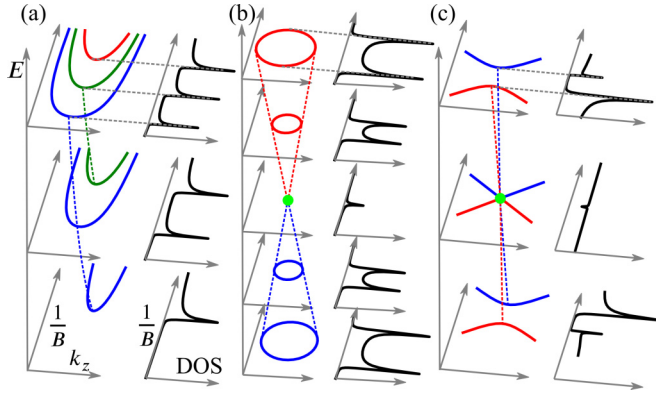


FIG. 1. Magnetic energy levels for a free-electron gas (a), and for topological nodal-line metals [(b), (c)]. Left of each panel: equienergy contours of energy-level surfaces in (B^{-1}, k_z) space, with distinct surfaces distinguished by color; right: corresponding density of states, regularized by a finite lifetime.

I. PROOF OF PRINCIPLE

We first present a minimal model of Landau-Dirac points with both τ_z and Tc_{2y} symmetries. At zero field, our effective-mass model describes two parabolic bands with opposite-sign masses:

$$H(\mathbf{k}) = [(k_x^2 + k_y^2)/2m - \varepsilon_0]\tau_3 + u_z k_z \tau_1 + u_x k_x. \quad (1)$$

$\varepsilon_0 > 0$ implies that the two bands overlap on the energy axis; however, level repulsion is absent in the $k_z = 0$ plane owing to τ_z symmetry: $\tau_3 H(\mathbf{k}) \tau_3 = H(k_x, k_y, -k_z)$. It follows that a zero-energy, nodal-line degeneracy encircles $\mathbf{k} = \mathbf{0}$ with radius $k_R = \sqrt{2m\varepsilon_0}$, supposing $u_x = 0$. If nonzero, the $u_x k_x$ term causes the nodal line to disperse with bandwidth $\Delta E = 2u_x k_R$. Thus, for a Fermi energy satisfying $|E_F| < \Delta E/2$, the Fermi surface comprises electron and hole pockets that interconnect like a linked sausage, as illustrated in Fig. 2(b). Close to either interconnection points (with $E_F = 0$), an effective Hamiltonian is attained by linearizing Eq. (1) around $\mathbf{k} = (0, \pm k_R, 0)$:

$$H_{\pm} = \pm u_y \delta k_y \tau_3 + u_z k_z \tau_1 + u_x k_x, \quad u_y = \sqrt{2\varepsilon_0/m}, \quad (2)$$

whose equienergy contours form a hyperbola depicted in the inset of Fig. 2(a).

Applying a magnetic field parallel to $-z$, the magnetic energy levels are eigenvalues of the Peierls-Onsager Hamiltonian $H(K_x, K_y, k_z)$, which is obtained by substituting (k_x, k_y) in the zero-field Hamiltonian [cf. Eq. (1)] by noncommuting operators satisfying $[K_y, K_x] = iB$ [42,43]. If B is much smaller than the \mathbf{k} area of both sausage-shaped pockets, the following semiclassical interpretation holds: The Lorentz force pushes electrons along trajectories indicated by arrows in Fig. 2(a). In the vicinity of both connection points [$\mathbf{k} = (0, \pm k_R, 0)$], interpacket tunneling occurs with the Landau-Zener probability [33,44–51]:

$$\rho^2 = e^{-2\pi\mu}, \quad \mu = S_{\square}/8B, \quad S_{\square} = 4v_z^2 k_z^2 / v_x v_y, \quad (3)$$

with S_{\square} being the rectangular area inscribed by the two hyperbolic arms [cf. inset of Fig. 2(a)]. By matching the Wentzel-Kramers-Brillouin (WKB) wave functions [52] at the tunneling regions (by the Landau-Zener connection for-

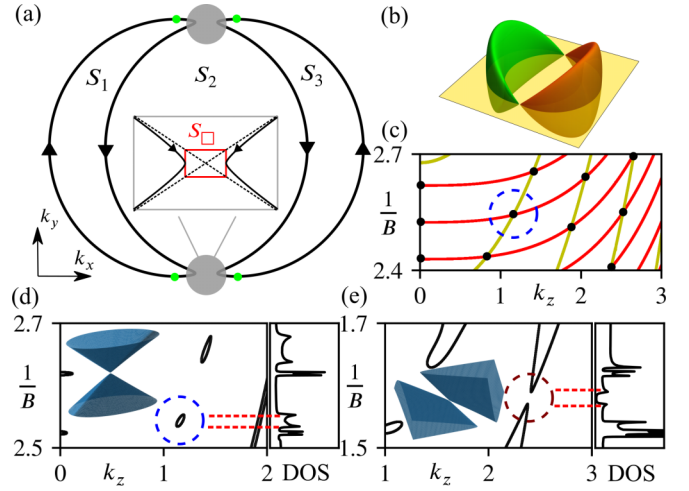


FIG. 2. For the minimal model in Eq. (1) with parameters $v_x = v_z = m = 1$ and $\varepsilon_0 = 10$, we plot the zero-energy, Fermi surface within the Brillouin zone in panel (b); a constant ($k_z = 0.4$) cross section of the same surface is shown in panel (a). Inset of panel (a): enlarged view of breakdown region. Landau-Fermi surfaces over (B^{-1}, k_z) are indicated by black dots and black lines in panels (c)–(e), for $E=0, 0.01, 0.95$ respectively. Right panels [(d) and (e)] plot the corresponding density of states (DOS) in arbitrary units. The diabolos in panel (d) [(e)] is the energy dispersion of the type I (resp., type II) Landau-Dirac cone encircled in blue (resp., brown).

mula [49]), we derive a quantization rule for the magnetic energy levels:

$$0 = Q(E, k_z, B^{-1}) = \cos X + \rho^2 \cos Y + \tau^2 \cos Z,$$

$$(X, Y, Z) = \frac{1}{2B} (S_1 - S_3, S_{12} + S_{23}, S_1 + S_3 + 4\omega B), \quad (4)$$

with $\tau^2 = 1 - \rho^2$ being the probability that an incoming electron “reflects” off the tunneling region with a different velocity. $\omega = \mu - \mu \ln \mu + \arg[\Gamma(i\mu)] + \pi/4$ is the phase acquired during this adiabatic reflection, with Γ being the Gamma function; S_1 (S_3) is the \mathbf{k} area of the left (right) sausage-shaped pocket, and $S_{12} := S_1 + S_2$ ($S_{23} := S_2 + S_3$) is the area of the left (right) circular trajectory linked by tunneling [cf. Fig. 2(a)].

For $k_z = \mu = 0$, Landau-Zener tunneling occurs with unit probability, and solutions of Eq. (4) describe independent cyclotron orbits over overlapping circles:

$$\cos X + \cos Y = 0 \Rightarrow S_{12,23}(E, 0)/B = 2\pi(n + 1/2). \quad (5)$$

The zero-energy solutions of Eq. (5) are doubly degenerate and lie at equidistant points on the vertical axis of Fig. 2(c), owing to the commensuration of areas: $S_{12}(0, k_z) = S_{23}(0, k_z)$, which derives from the effective-mass Hamiltonian in Eq. (1).

There is no unique semiclassical trajectory in the intermediate tunneling regime with nonzero, finite $\mu \propto k_z^2$. We focus on a class of solutions contained in certain hypersurfaces in (E, k_z, B^{-1}) space (r space, in short), defined by $X(r)/\pi \in 2\mathbb{Z}$ and $2\mathbb{Z} + 1$. Whether even or odd, $\cos X$ is extremized to ± 1 , and hence this class of solutions satisfy $\cos Y = \cos Z = \mp \cos X$. These two constraints (within a two-dimensional hypersurface) can only be satisfied at isolated points, denoted by $\{\bar{r}\}$. Such points lying within the $(X = 0)$ hypersurface

are illustrated as black dots in Fig. 2(c); note the ($X = 0$) hypersurface is just the $E = 0$ plane owing to the just-mentioned commensuration condition, and the black dots lie at the intersections of red lines (defined by $\cos Y = -1$) and yellow lines ($\cos Z = -1$).

Moving off a hypersurface in the normal (or antinormal) direction, each point solution evolves into an ellipse, as illustrated for $E = 0.01$ in Fig. 2(d). To prove that \bar{r} is a diabolical point, apply that \bar{r} is an extremal point for each of $\{\cos X, \cos Y, \cos Z\}$. Consequently, for any solution of the quantization rule that deviates from \bar{r} by small $\delta r = (\delta E, \delta k_z, \delta B^{-1})$, $0 = Q(\bar{r} + \delta r) - Q(\bar{r})$, with the right-hand side quadratic in δr to the lowest order. Solving this quadratic equation for the Landau-level dispersion,

$$\begin{aligned} \delta E &= (-b \pm \sqrt{b^2 - 4ac})/2a, \quad a = X_E^2 - \rho^2 Y_E^2 - \tau^2 Z_E^2, \\ b &= [2X_E(\delta k_z X_z + \delta B^{-1} X_{B^{-1}})] - \rho^2[X \rightarrow Y] - \tau^2[X \rightarrow Z], \\ c &= [(\delta k_z X_z + \delta B^{-1} X_{B^{-1}})^2] - \rho^2[X \rightarrow Y] - \tau^2[X \rightarrow Z]. \end{aligned}$$

$X_{E, k_z, B^{-1}}$ denotes the partial derivative of X with respect to (E, k_z, B^{-1}) , as evaluated at \bar{r} ; $[X \rightarrow Y]$ denotes the substitution of X with Y in the square-bracketed expression on the same line. Since the quantity under the square root is quadratic in $(\delta k_z, \delta B^{-1})$, the solution in $(\delta k_z, \delta B^{-1})$ space generically forms a diabolo with vertex at \bar{r} .

The perturbative stability of Landau-Dirac points is guaranteed by $T_{C_{2y}}$ symmetry: $H(K_x, K_y, k_z)^* = H(K_x, -K_y, k_z)$. Given this antiunitary constraint, a standard generalization [53] of the von Neumann–Wigner theorem [1] states that the codimension of an eigenvalue degeneracy is two, implying degeneracies are perturbatively stable in the two-dimensional (B^{-1}, k_z) space. The Landau-Dirac points at $k_z = 0$ are doubly protected by τ_z symmetry, because each such point is a crossing between levels in distinct eigenspaces of τ_3 .

II. TYPE-II LANDAU-DIRAC POINTS

While the ($X = 0$) hypersurface is the $E = 0$ plane, ($X = \pi j$) hypersurfaces are increasingly dispersive for larger $|j|$. With sufficient dispersion, the conical axis tilts away from the energy axis, such that the diabolo [centered at $(\bar{E}, \bar{k}_z, \bar{B}^{-1})$] intersects the $E = \bar{E}$ plane on open lines; such a *type-II Landau-Dirac point* occurs if and only if $ac < 0$ on any segment of a circle encircling the diabolical point. A type-II point lying on the $X = 6\pi$ hypersurface is illustrated in Fig. 2(e).

An isolated, type-I point is distinguishable from type II by the Fermi-level density of states (DOS). The intersection of a magnetic band with the Fermi level defines a *Landau-Fermi surface* in $(1/B, k_z)$ space; in the type-I case, the Landau-Fermi surface is deformable to a circle, and can be parametrized by a multivalued function $B^{-1}(k_z)$ with two extrema. At each extremum, the DOS has a van Hove singularity that is left-right asymmetric, being proportional to $[\pm(B^{-1} - B_0^{-1})]^{-1/2}$ on one side of the singularity but not the other. (Such left-right asymmetry is routinely measurable in thermodynamic and galvanomagnetic experiments [54–56].) Figure 1 illustrates that the inverse-square-root “tails” (in a type-I scenario) trail toward each other, resembling the helm of Batman; conversely, type-II tails trail apart, like anti-Batman. For our minimal model in Eq. (1), we plot

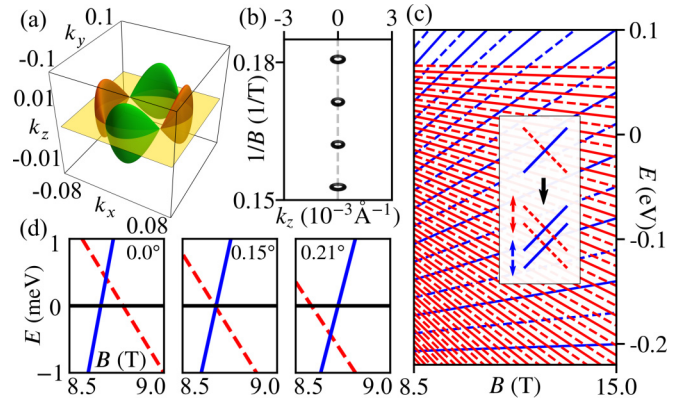


FIG. 3. For a $k \cdot p$ model [57] of CaP_3 without spin-orbit coupling, we plot (a) the Fermi surface, (b) Landau-Fermi surface, and (c) Landau-level dispersion at $k_z = 0$ and B parallel to z . Panel (d) shows the dispersion of a specific Landau-Dirac point, for B tilted within the xz plane by angles $\theta_B = 0^\circ, 0.15^\circ, 0.21^\circ$, with the electron density fixed throughout. Inset of panel (c) illustrates a spin-split Landau-Dirac point.

the DOS in the right panels of Figs. 2(d) and 2(e), with the correspondence between Batman peaks and type-I Landau-Fermi surfaces [resp. anti-Batman and type II] indicated by red dashed lines in Fig. 2(d) [resp. Fig. 2(e)]. Unlike conventional peaks in Schubnikov–de Haas–van Alphen oscillations, Batman peaks associated to quantum tunneling are generally *nonperiodic* in $1/B$; the width of the Batman helm is likewise *not* attributable to the area of any k loop in the graph.

III. MATERIAL CASE STUDIES

The Landau-Dirac phenomenology potentially manifests in a number of topological-metallic candidates: CaAs_3 [58], CaP_3 [57], SrP_3 [57], and Ca_3P_2 [59,60], each of which has a Fermi surface enclosing a single, circular nodal line—just like our minimal model. For concreteness, we pick $P\bar{1}$ -symmetric [61] CaX_3 ($X = \text{As}, \text{P}$) for our final case study. Its point group is generated solely by the spatial inversion i . CaX_3 's nodal line is predicted [57,58] to be centered at an inversion-invariant wavevector on the BZ boundary, and encircles an area $\lesssim 1/50$ the areal dimension of the BZ—this allows for an accurate description by an effective-mass Hamiltonian $H(\mathbf{k}) = \sum_{i=0}^3 d_i(\mathbf{k})\tau_i$, with τ_0 being the identity matrix; the two-by-two matrix structure reflects our (present) ignorance of the weak spin-orbit interaction.

Our effective-mass parameters (detailed in the Supplemental Material [62]) are chosen such that the Fermi surface consists of four interconnected pockets (two electron-like and two hole-like), as has been predicted for CaX_3 [57,58]. Owing to i symmetry [$\tau_3 H(\mathbf{k}) \tau_3 = H(-\mathbf{k})$] and time-reversal symmetry (represented by complex conjugation), momentum coordinates can be chosen such that the inter-pocket connections lie in the $k_z = 0$ plane [cf. Fig. 3(a)] and $[H(k_x, k_y, k_z = 0), \tau_3] = 0$. This $U(1) \times U(1)$ symmetry encodes the nonmixing of orbitals indexed by $\langle \tau_3 \rangle = \pm 1$.

The corresponding Landau levels (restricted to $k_z = 0$) are plotted in Fig. 3(c), with blue (red) lines indicating $\langle \tau_3 \rangle = 1$ ($\langle \tau_3 \rangle = -1$). For either $\langle \tau_3 \rangle$, the i eigenvalue alternates be-

tween adjacent levels [23], as illustrated by alternating solid (i-even) and dashed (i-odd) lines. Half of the Landau-Dirac points in Fig. 3(c) are i-protected crossings between solid and dashed lines; the other half are protected by $U(1) \times U(1)$ symmetry but not by i . For small $k_z \neq 0$, the four sausage links in Fig. 3(a) disconnect; electron dynamics in the vicinity of the four disconnected links is again of the Landau-Zener type, with tunneling probability $\exp(-2\pi\mu)$. The resultant Landau-Fermi surface form closed lobes encircling the type-I Landau-Dirac points at $k_z = 0$, as shown in Fig. 3(b).

Though our analysis has assumed a specific field orientation, half the crossings in Fig. 3(c) are perturbatively stable against tilting of the field, because i symmetry is maintained for any field orientation; the other half that relies on $U(1) \times U(1)$ symmetry will destabilize.

We have thus far neglected spin in the CaX_3 study. Because the intrinsic Zeeman and spin-orbit interactions maintain i symmetry, each spin-degenerate Landau level perturbatively splits in energy, converting a single, spin-degenerate, i -protected Landau-Dirac point into four, spin-nondegenerate, i -protected Landau-Dirac points, as illustrated in Fig. 3(c). Nonperturbatively, we expect the Landau-Dirac cones to persist so long as the spin-orbit energy is less than the dispersion bandwidth of the nodal line [cf. ΔE below Eq. (1)]; this is the regime where quantum tunneling remains relevant.

IV. EXPERIMENTAL DIAGNOSTICS

The experimental observation of Batman peaks in the magnetoresistance would be suggestive but not conclusive of a type-I Landau-Dirac cone. One must further demonstrate that both peaks originate from a single Landau-Fermi surface that is topologically equivalent to a circle in $(1/B, k_z)$ space [cf. Fig. 1(b)]. This relies on our ability to map out the entire Landau-Fermi surface, which we propose to accomplish by *angle-dependent ultrasound attenuation*. Our proposal generalizes existing ultrasound methodology [54,63,64] to measure “giant quantum oscillations” [65] in the $(1/B)$ -dependent attenuation coefficient, for which the angle between sound wave vector and B field remains *fixed*. We propose here to ignore these oscillations and instead track *individual* peaks by varying both the B magnitude and the sound-wave vector orientation, with fixed B orientation.

When an electronic quasiparticle in a magnetic energy band [with dispersion $E_n(k_z, B)$] absorbs an acoustic phonon [with typical wavenumber $|\mathbf{q}| \approx (5 \mu\text{m})^{-1}$], inter-Landau-level transitions are forbidden for B large enough that $|E_{n+1} - E_n| > 0.1 \text{ meV}$. This inequality holds assuming that the magnetic velocity in the Taylor expansion

$$E_n(k_z + q_z, B) = E_n(k_z, B) + v_n(k_z, B)q_z + \frac{q_z^2}{2m_n(k_z, B)} + \dots$$

satisfies $|v_n| \leq c/100$, and the magnetic mass $m_n > m_e/1000$ with m_e being the free-electron mass. Energy-momentum conservation requires that resonant sound absorption occurs only if the electron “rides the surf” of the sound-wave fronts [54,64], i.e., the \mathbf{q} -parallel component of the magnetic velocity ($v_n \mathbf{B}/|\mathbf{B}|$) equals the sound speed s :

$$v_n(k_z, B_n) \cos(\theta) \approx s(\mathbf{q}/|\mathbf{q}|), \quad \cos \theta = \frac{\mathbf{B}}{|\mathbf{B}|} \cdot \frac{\mathbf{q}}{|\mathbf{q}|}. \quad (6)$$

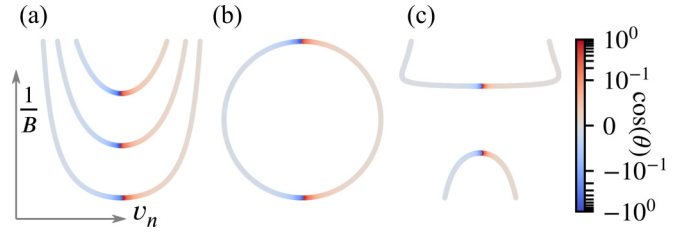


FIG. 4. For the highest equienergy contours of Figs. 1(a)–1(c), we plot $1/B$ vs the field-parallel Fermi velocity $v_n = dE_n/dk_z$ in panels (a)–(c), respectively. The color of the plotted lines indicate the direction cosine $\cos(\theta) \in [-1, 1]$ (of sound wave vector relative to B field) where resonant, ultrasound absorption occurs. We have assumed an isotropic sound speed s satisfying $s/\max(|v_n|) = 1/100$.

Pauli’s exclusion principle requires that we evaluate v_n at $B = B_n$ where the n th Landau level crosses the Fermi level. Fixing $B = B_n$ and varying θ , resonant absorption occurs at an angle-dependent electronic wave number $k_{z,n} = k_z(\cos \theta, B_n, s)$ satisfying Eq. (6). By varying $\theta \in [0, \pi]$, $k_{z,n}$ covers essentially the entire Landau-Fermi surface; only a tiny fraction ($\sim s/\max(|v_n|) \lesssim 10^{-2}$) of the surface is missed for k_z values where $v_n \lesssim s$, and Eq. (6) cannot be satisfied. In practice, θ is varied by gluing piezoelectric transducers [63] to multiple crystal facets cut by wire or focused ion beam [66], with the facet orientation determined by x-ray diffraction. Figure 4 illustrates how this technique is able, in principle, to distinguish the Landau-Fermi surfaces associated to free electrons, type-I and type-II Landau-Dirac cones: The reconstructed surfaces over $(1/B, v_n)$ are topologically equivalent to the Landau-Fermi surfaces over $(1/B, k_z)$.

We have assumed in Fig. 4 the generic scenario in which the Landau-Dirac point lies away from the Fermi level. Otherwise, inter-Landau-level transitions may occur with Eq. (6) failing to hold. Two tunable parameters are needed to bring an i - or τ_z -protected Landau-Dirac point to the Fermi level, e.g., by tuning B^{-1} , the two Landau levels (closest to the Fermi level) can be made to cross; by tuning the B -tilt angle θ_B , such crossing can be brought to the Fermi level, as illustrated in Fig. 3(d) for the CaX_3 model.

To directly diagnose a Landau-Dirac *point*, we propose that the frequency onset of optical absorption *linearly* evolves to zero as a function of θ_B . Such an optical transition between Landau levels of distinct i representations is allowed by the dipole selection rule [67]. Optical experiments in the far-infrared, submillimeter-wavelength regime [68–70] have a penetration depth $\lambda \approx 100 \text{ nm}$ in many metals [71] λ greatly exceeding the magnetic length $[25 \text{ nm}/\sqrt{B(T)}]$ for $B \approx 10 \text{ T}$ allows for optical excitations to directly reflect bulk, inter-Landau-level transitions.

V. DISCUSSION

We have shown how the diabolical point in solid-state, magnetic energy levels originates from quantum tunneling; an individual Landau-Dirac point is topologically irremovable if certain magnetic space-group symmetries are preserved. Topological nodal-line metals provide an ideal experimental platform to realize Landau-Dirac points. *Ab initio*

calculations have predicted that CaX_3 is either a band-inverted topological metal, or can be band inverted under lattice compression [57,58,72]. The existence of a nodal line in CaAs_3 is as yet inconclusive, but would be corroborated by observing the Landau-Dirac phenomenology proposed in this work.

Future investigations would determine if a similar phenomenology exists for two other topological-nodal-line material candidates, which host more complicated Fermi surfaces than the present study: (a) SrAs_3 has an experimentally evidenced [73–75], nodal-line degeneracy, and (b) the square-net compound ZrSiS is known to undergo magnetic breakdown [76]. While SrAs_3 is chemically similar to CaAs_3 , the former has an additional, twofold rotational symmetry that protects nodal-line degeneracies in (B^{-1,k_z}) space, if the field is oriented along the twofold axis.

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- [1] J. von Neumann and E. Wigner, On the behavior of eigenvalues in adiabatic processes, *Phys. Z.* **30**, 467 (1929).
- [2] E. Teller, The crossing of potential surfaces, *J. Phys. Chem.* **41**, 109 (1937).
- [3] M. V. Berry, Semiclassical mechanics of regular and irregular motion, in *Les Houches Lecture Series, Session XXXVI*, edited by G. Iooss, R. H. G. Helleman, and R. Strora (North-Holland, Amsterdam, 1983), pp. 171–271.
- [4] M. V. Berry and M. Wilkinson, Diabolical points in the spectra of triangles, *Proc. R. Soc. London, Ser. A* **392**, 15 (1984).
- [5] W. Hamilton, Third supplement to an essay on the theory of systems of rays, *Trans. R. Irish Acad.* **17**, 1 (1837).
- [6] M. Berry and M. Jeffrey, Conical diffraction: Hamilton's diabolical point at the heart of crystal optics, in *Progress in Optics*, edited by E. Wolf (Elsevier, Amsterdam, 2007), Vol. 50, pp. 13–50.
- [7] M. V. Berry and M. R. Dennis, The optical singularities of birefringent dichroic chiral crystals, *Proc. R. Soc. London Ser. A* **459**, 1261 (2003).
- [8] G. Herzberg and H. C. Longuet-Higgins, Intersection of potential energy surfaces in polyatomic molecules, *Discuss. Faraday Soc.* **35**, 77 (1963).
- [9] C. A. Mead and D. G. Truhlar, On the determination of Born-Oppenheimer nuclear motion wave functions including complications due to conical intersections and identical nuclei, *J. Chem. Phys.* **70**, 2284 (1979).
- [10] L. S. Cederbaum, R. S. Friedman, V. M. Ryabov, and N. Moiseyev, Conical Intersections and Bound Molecular States Embedded in the Continuum, *Phys. Rev. Lett.* **90**, 013001 (2003).
- [11] A. Farhan, L. Canto, J. Rasmussen, and P. Ring, Form factors for two-nucleon transfer in the diabolical region of rotating nuclei, *Nucl. Phys. A* **597**, 387 (1996).
- [12] A. Ferretti, A. Lami, and G. Villani, Transition probability due to a conical intersection: On the role of the initial conditions and of the geometric setup of the crossing surfaces, *J. Chem. Phys.* **111**, 916 (1999).
- [13] H. Nielsen and M. Ninomiya, The Adler-Bell-Jackiw anomaly and Weyl fermions in a crystal, *Phys. Lett. B* **130**, 389 (1983).
- [14] P. Hořava, Stability of Fermi Surfaces and K Theory, *Phys. Rev. Lett.* **95**, 016405 (2005).
- [15] K. S. Novoselov, A. K. Geim, S. V. Morozov, D. Jiang, M. I. Katsnelson, I. V. Grigorieva, S. V. Dubonos, and A. A. Firsov, Two-dimensional gas of massless Dirac fermions in graphene, *Nature (London)* **438**, 197 (2005).
- [16] X. Wan, A. M. Turner, A. Vishwanath, and S. Y. Savrasov, Topological semimetal and Fermi-arc surface states in the electronic structure of pyrochlore iridates, *Phys. Rev. B* **83**, 205101 (2011).
- [17] G. B. Halasz and L. Balents, Time-reversal invariant realization of the Weyl semimetal phase, *Phys. Rev. B* **85**, 035103 (2012).
- [18] A. A. Soluyanov, D. Gresch, Z. Wang, Q. Wu, M. Troyer, X. Dai, and B. A. Bernevig, Type-II Weyl semimetals, *Nature (London)* **527**, 495 (2015).
- [19] C. H. Kane and E. J. Mele, Quantum Spin Hall Effect in Graphene, *Phys. Rev. Lett.* **95**, 226801 (2005).
- [20] L. Fu, C. L. Kane, and E. J. Mele, Topological Insulators in Three Dimensions, *Phys. Rev. Lett.* **98**, 106803 (2007).
- [21] J. E. Moore and L. Balents, Topological invariants of time-reversal-invariant band structures, *Phys. Rev. B* **75**, 121306(R) (2007).
- [22] R. Roy, Topological phases and the quantum spin Hall effect in three dimensions, *Phys. Rev. B* **79**, 195322 (2009).
- [23] L. D. Landau and E. M. Lifshitz, *Quantum Mechanics* (Elsevier, Singapore, 2007).
- [24] M. V. Berry, Quantal phase factors accompanying adiabatic changes, *Proc. R. Soc. London Ser. A* **392**, 45 (1984).
- [25] L. Onsager, Interpretation of the de Haas-van Alphen effect, *Philos. Mag.* **43**, 1006 (1952).
- [26] L. M. Lifshitz and A. Kosevich, On the theory of the de Haas-van Alphen effect for particles with an arbitrary dispersion law, *Dokl. Akad. Nauk SSSR* **96**, 963 (1954).
- [27] L. M. Roth, Semiclassical theory of magnetic energy levels and magnetic susceptibility of Bloch electrons, *Phys. Rev.* **145**, 434 (1966).
- [28] J. B. Keller, Corrected Bohr-Sommerfeld quantum conditions for nonseparable systems, *Ann. Phys. (NY)* **4**, 180 (1958).

- [29] G. P. Mikitik and Y. V. Sharlai, Manifestation of Berry's Phase in Metal Physics, *Phys. Rev. Lett.* **82**, 2147 (1999).
- [30] M.-C. Chang and Q. Niu, Berry phase, hyperorbits, and the Hofstadter spectrum: Semiclassical dynamics in magnetic Bloch bands, *Phys. Rev. B* **53**, 7010 (1996).
- [31] M. H. Cohen and L. M. Falicov, Magnetic Breakdown in Crystals, *Phys. Rev. Lett.* **7**, 231 (1961).
- [32] M. Y. Azbel, Quasiclassical quantization in the neighborhood of singular classical trajectories, *J. Exp. Theor. Phys.* **12**, 891 (1961).
- [33] E. I. Blount, Bloch electrons in a magnetic field, *Phys. Rev.* **126**, 1636 (1962).
- [34] A. B. Pippard, Quantization of coupled orbits in metals, *Proc. R. Soc. London Ser. A* **270**, 1 (1962).
- [35] W. G. Chambers, Magnetic breakdown: Effective hamiltonian and de Haas-van Alphen effect, *Phys. Rev.* **149**, 493 (1966).
- [36] A. A. Burkov, M. D. Hook, and L. Balents, Topological nodal semimetals, *Phys. Rev. B* **84**, 235126 (2011).
- [37] Y. Chen, Y. Xie, S. A. Yang, H. Pan, F. Zhang, M. L. Cohen, and S. Zhang, Nanostructured carbon allotropes with Weyl-like loops and points, *Nano Lett.* **15**, 6974 (2015).
- [38] T. Bzdušek, Q. Wu, A. Rüegg, M. Sigrist, and A. A. Soluyanov, Nodal-chain metals, *Nature (London)* **538**, 75 (2016).
- [39] C.-K. Chiu and A. P. Schnyder, Classification of reflection-symmetry-protected topological semimetals and nodal superconductors, *Phys. Rev. B* **90**, 205136 (2014).
- [40] B.-J. Yang, T. A. Bojesen, T. Morimoto, and A. Furusaki, Topological semimetals protected by off-centered symmetries in nonsymmorphic crystals, *Phys. Rev. B* **95**, 075135 (2017).
- [41] C. Fang, H. Weng, X. Dai, and Z. Fang, Topological nodal line semimetals, *Chin. Phys. B* **25**, 117106 (2016).
- [42] R. Peierls, Zur theorie des diamagnetismus von leitungselektronen, *Z. Phys.* **80**, 763 (1933).
- [43] J. M. Luttinger, The effect of a magnetic field on electrons in a periodic potential, *Phys. Rev.* **84**, 814 (1951).
- [44] C. Zener and R. H. Fowler, Non-adiabatic crossing of energy levels, *Proc. R. Soc. London Ser. A* **137**, 696 (1932).
- [45] A. Slutskin, Dynamics of conduction electrons under magnetic breakdown conditions, *J. Exp. Theor. Phys.* **26**, 474 (1968).
- [46] M. Kaganov and A. Slutskin, Coherent magnetic breakdown, *Phys. Rep.* **98**, 189 (1983).
- [47] T. E. O'Brien, M. Diez, and C. W. J. Beenakker, Magnetic Breakdown and Klein Tunneling in a Type-II Weyl Semimetal, *Phys. Rev. Lett.* **116**, 236401 (2016).
- [48] A. Alexandradinata and L. Glazman, Geometric Phase and Orbital Moment in Quantization Rules for Magnetic Breakdown, *Phys. Rev. Lett.* **119**, 256601 (2017).
- [49] A. Alexandradinata and L. Glazman, Semiclassical theory of Landau levels and magnetic breakdown in topological metals, *Phys. Rev. B* **97**, 144422 (2018).
- [50] C. Wang, W. Duan, L. Glazman, and A. Alexandradinata, Landau quantization of nearly degenerate bands and full symmetry classification of Landau level crossings, *Phys. Rev. B* **100**, 014442 (2019).
- [51] M. Breitzkreuz, N. Bovenzi, and J. Tworzydło, Phase shift of cyclotron orbits at type-I and type-II multi-Weyl nodes, *Phys. Rev. B* **98**, 121403(R) (2018).
- [52] G. E. Zil'berman, Behavior of an electron in a periodic electric and a uniform magnetic field, *J. Exp. Theor. Phys.* **5**, 208 (1957).
- [53] A. Alexandradinata and J. Höller, No-go theorem for topological insulators and high-throughput identification of Chern insulators, *Phys. Rev. B* **98**, 184305 (2018).
- [54] D. Shoenberg, *Magnetic Oscillations in Metals* (Cambridge University Press, Cambridge, UK, 1984).
- [55] J. S. Dhillon and D. Shoenberg, The de Haas-van Alphen effect III. Experiments at fields up to 32KG, *Philos. Trans. R. Soc. London Ser. A* **248**, 1 (1955).
- [56] C. Guo, A. Alexandradinata, C. Putzke, F.-R. Fan, S. Zhang, Q. Wu, O. V. Yazyev, K. R. Shirer, M. D. Bachmann, E. D. Bauer, F. Ronning, C. Felser, Y. Sun, and P. J. W. Moll, Temperature dependence of quantum oscillations from non-parabolic dispersions, *Nat. Commun.* **12**, 6213 (2021).
- [57] Q. Xu, R. Yu, Z. Fang, X. Dai, and H. Weng, Topological nodal line semimetals in the CaP₃ family of materials, *Phys. Rev. B* **95**, 045136 (2017).
- [58] Y. Quan, Z. P. Yin, and W. E. Pickett, Single Nodal Loop of Accidental Degeneracies in Minimal Symmetry: Triclinic CaAs₃, *Phys. Rev. Lett.* **118**, 176402 (2017).
- [59] L. S. Xie, L. M. Schoop, E. M. Seibel, Q. D. Gibson, W. Xie, and R. J. Cava, A new form of Ca₃P₂ with a ring of dirac nodes, *APL Mater.* **3**, 083602 (2015).
- [60] Y.-H. Chan, C.-K. Chiu, M. Y. Chou, and A. P. Schnyder, Ca₃P₂ and other topological semimetals with line nodes and drumhead surface states, *Phys. Rev. B* **93**, 205132 (2016).
- [61] W. Dahlmann and H. G. v. Schnering, CaP₃, ein neues calciumphosphid, *Naturwissenschaften* **60**, 518 (1973).
- [62] See Supplemental Material, which cites Refs. [23,25,27–29,44,46,49,50,54,57,64,64,65,65,77–88], at <http://link.aps.org/supplemental/10.1103/PhysRevB.105.045141> for more details about angle-dependent ultrasonic attenuation, quantization rules, effective mass model of candidate materials, and a discussion about coexisting Fermi pockets.
- [63] A. M. Toxen and S. Tansal, Giant oscillations in the magnetoacoustic attenuation of bismuth, *Phys. Rev.* **137**, A211 (1965).
- [64] Y. Shapira, Acoustic wave propagation in high magnetic fields, in *Principles and Methods*, Physical Acoustics Vol. 5, edited by W. P. Mason (Academic Press, San Diego, 1968), pp. 1–58.
- [65] V. L. Gurevich, V. G. Skobov, and Y. A. Firsov, Giant quantum oscillations in the acoustical absorption by a metal in a magnetic field, *J. Exp. Theor. Phys.* **13**, 552 (1961).
- [66] P. J. Moll, Focused ion beam microstructuring of quantum matter, *Annu. Rev. Condens. Matter Phys.* **9**, 147 (2018).
- [67] W. Zawadzki, Intraband and interband magneto-optical transitions in semiconductors, in *Landau Level Spectroscopy*, edited by G. Landwehr and E. I. Rashba (Elsevier, North-Holland, Amsterdam, 1991), p. 485.
- [68] M. A. Ordal, R. J. Bell, R. W. Alexander, L. L. Long, and M. R. Query, Optical properties of Au, Ni, and Pb at submillimeter wavelengths, *Appl. Opt.* **26**, 744 (1987).
- [69] H.-J. Hagemann, W. Gudat, and C. Kunz, Optical constants from the far infrared to the x-ray region: Mg, Al, Cu, Ag, Au, Bi, C, and Al₂O₃, *J. Opt. Soc. Am.* **65**, 742 (1975).
- [70] D. Grischkowsky, S. Keiding, M. van Exter, and C. Fittinger, Far-infrared time-domain spectroscopy with terahertz beams of dielectrics and semiconductors, *J. Opt. Soc. Am. B* **7**, 2006 (1990).
- [71] Optical data and references are available at <https://refractiveindex.info>.

- [72] J. Li, L.-X. Zhao, Y.-Y. Wang, X.-M. Wang, C.-Y. Ma, W.-L. Zhu, M.-R. Gao, S. Zhang, Z.-A. Ren, and G.-F. Chen, Transport properties of topological nodal-line semimetal candidate CaAs_3 under hydrostatic pressure, *Chin. Phys. B* **28**, 046202 (2019).
- [73] S. Li, Z. Guo, D. Fu, X.-C. Pan, J. Wang, K. Ran, S. Bao, Z. Ma, Z. Cai, R. Wang, R. Yu, J. Sun, F. Song, and J. Wen, Evidence for a Dirac nodal-line semimetal in SrAs_3 , *Sci. Bull.* **63**, 535 (2018).
- [74] L. An, X. Zhu, W. Gao, M. Wu, W. Ning, and M. Tian, Chiral anomaly and nontrivial Berry phase in the topological nodal-line semimetal SrAs_3 , *Phys. Rev. B* **99**, 045143 (2019).
- [75] M. M. Hosen, G. Dhakal, B. Wang, N. Poudel, K. Dimitri, F. Kabir, C. Sims, S. Regmi, K. Gofryk, D. Kaczorowski, A. Bansil, and M. Neupane, Experimental observation of drum-head surface states in SrAs_3 , *Sci. Rep.* **10**, 2776 (2020).
- [76] S. Pezzini, M. Van Delft, L. Schoop, B. Lotsch, A. Carrington, M. Katsnelson, N. Hussey, and S. Wiedmann, Unconventional mass enhancement around the Dirac nodal loop in ZrSiS , *Nat. Phys.* **14**, 178 (2018).
- [77] A. I. Akhiezer, M. I. Kaganov, and G. L. Liubarskii, Ultrasonic absorption in metals, *J. Exp. Theor. Phys.* **5**, 685 (1957).
- [78] Y. Sawada, E. Burstein, and L. Testardi, Determination of the Energy Band Parameters of Bismuth by Giant Quantum Attenuation of Sound Waves, in *Proceedings of the International Conference on the Physics of Semiconductors, Kyoto, 1966* (Physical Society of Japan, 1966).
- [79] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Thomson Learning, Boston, MA, 1976).
- [80] V. G. Skobov, Quantum theory of sound absorption by metals in a magnetic field, *J. Exp. Theor. Phys.* **13**, 1014 (1961).
- [81] L. M. Lifshitz and A. Kosevich, Theory of magnetic susceptibility in metals at low temperatures, *J. Exp. Theor. Phys.* **2**, 636 (1956).
- [82] L. M. Falicov and H. Stachowiak, Theory of the de Haas–van Alphen effect in a system of coupled orbits. application to magnesium, *Phys. Rev.* **147**, 505 (1966).
- [83] J. Zak, Magnetic translation group, *Phys. Rev.* **134**, A1602 (1964).
- [84] E. Brown, Bloch electrons in a uniform magnetic field, *Phys. Rev.* **133**, A1038 (1964).
- [85] J. P. Perdew, K. Burke, and M. Ernzerhof, Generalized Gradient Approximation Made Simple, *Phys. Rev. Lett.* **77**, 3865 (1996).
- [86] J. Heyd, G. E. Scuseria, and M. Ernzerhof, Hybrid functionals based on a screened Coulomb potential, *J. Chem. Phys.* **118**, 8207 (2003).
- [87] G. Kresse and J. Furthmüller, Efficient iterative schemes for *ab initio* total-energy calculations using a plane-wave basis set, *Phys. Rev. B* **54**, 11169 (1996).
- [88] G. Kresse and D. Joubert, From ultrasoft pseudopotentials to the projector augmented-wave method, *Phys. Rev. B* **59**, 1758 (1999).