Magnetic-Field-Induced Relativistic Properties in Type-I and Type-II Weyl Semimetals

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We investigate Weyl semimetals with tilted conical bands in a magnetic field. Even when the cones are overtitled (type-II Weyl semimetal), Landau-level quantization can be possible as long as the magnetic field is oriented close to the tilt direction. Most saliently, the tilt can be described within the relativistic framework of Lorentz transformations that give rise to a rich spectrum, displaying new transitions beyond the usual dipolar ones in the optical conductivity. We identify particular features in the latter that allow one to distinguish between semimetals of different types.

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The discovery of massless ultrarelativistic electrons in graphene [1,2] has triggered a tremendous interest in novel types of semimetallic phases in condensed-matter systems [3–5]. A particularly intriguing class is that of electronic systems with tilted Dirac cones that were first investigated in the framework of Lorentz transformations that give rise to a rich spectrum, displaying new transitions beyond the usual dipolar ones in the optical conductivity. We identify particular features in the latter that allow one to distinguish between semimetals of different types.

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Indeed, one may naturally ask what happens when the Dirac cones are overtitled such that the original reciprocal isoenergy trajectories are no longer closed ellipses but open hyperbolas [7]. In the presence of a magnetic field, the tilted Dirac cones may be characterized with the help of Lorentz transformations. As we discuss in more detail below, this can be achieved if one identifies the tilt with an effective electric field \( \mathcal{E} \) that was investigated in a covariant description by Lukose et al. [8]. This hints at an intimate relation between the tilt of the Dirac cones and relativistic transformations that was later investigated in the framework of magnetotransport [9] and magneto-optics [10].

Indeed, one may naturally ask what happens when the Dirac cones are overtitled such that the original reciprocal isoenergy trajectories are no longer closed ellipses but open hyperbolas [7]. In the presence of a magnetic field, the tilted Dirac cones may be characterized with the help of Lorentz transformations. As we discuss in more detail below, this can be achieved if one identifies the tilt with an effective electric field \( \mathcal{E} \). Below the critical tilt, we are confronted with a “weak” electric field that allows for a Lorentz boost to a frame of reference where \( \mathcal{E} \) effectively vanishes. In this so-called magnetic regime [11], the electronic orbits are then still closed (cyclotron orbits) and their energy is quantized into Landau levels (LLs) [12]. In contrast, such a boost is not possible for overtitled cones that correspond to a “strong” electric field. Via a Lorentz transformation, one can now simply find a frame of reference where the \( B \) field vanishes. This electric regime is characterized by open orbits that prevent LL quantization. Whereas overtitled cones have not been found in 2D materials, following the proposal by Soluyanov et al. [13], several three-dimensional (3D) systems have been identified during the last months as possible candidates for representing such a phase [14–17]. Furthermore, these phases, coined type-II Weyl semimetals (WSM), have been classified from a topological point of view [18,19].

In the present Letter, we show that the above classification needs to be revisited in 3D systems that present a remarkably rich behavior. Indeed, we find that a type-II WSM can undergo a transition from the magnetic to the electric regime as a function of the angle between the magnetic field and the tilt direction. Whereas the electric regime is at first sight the natural regime of a type-II WSM, the latter can nevertheless show LL quantization—the tilt is then most prominent in the direction of the \( B \) field, and the original overtilt is well represented by a one-dimensional band in the latter direction. This situation needs to be contrasted with that of at type-I WSM that is always in the magnetic regime regardless of the \( B \)-field direction. However, one can, at least in principle, induce transitions between WSM of the two different types by the application of an additional electric field with a nonzero component perpendicular to the \( B \) field. Finally, we investigate in detail the magneto-optical signatures in the magnetic regime, which allow for a distinction between type-I and type-II WSM. Most saliently, we find, similarly to tilted Dirac cones in 2D materials [10], that a magnetic field applied in a direction different from the tilt yields magneto-optical transitions beyond the usual dipolar ones that couple LLs with adjacent indices, \( n \to (n \pm 1) \).

Tilted Dirac cones in 3D systems can be modeled conveniently by the Hamiltonian

\[
H = \mathbf{\omega}_0 \cdot \mathbf{k} + \sum_{\mu=1}^{3} v_\mu k_\mu \hat{\sigma}_\mu, \tag{1}
\]

in terms of the three Pauli matrices \( \hat{\sigma}_\mu (\mu = 1, 2, 3) \) and the anisotropic Fermi velocities \( v_\mu \). Here and in the following, we use a system of units where \( \hbar = 1 \). Furthermore, we combine the tilt velocities \( \mathbf{\omega}_0 = (\omega_{0x}, \omega_{0y}, \omega_{0z}) \) into the tilt parameter vector
which allows us to distinguish a type-I WSM \(|t| < 1\) from a type-II WSM \(|t| > 1\), in analogy with the 2D case [7]. In order to account for a magnetic field in the \(z\)-direction, we use the Peierls substitution \(\mathbf{k} \rightarrow (q_x, q_y, k_z)\) with \(q_{x/y} = k_{x/y} + eA_{x/y}(\mathbf{r})\) and \(\mathbf{B} = \nabla \times \mathbf{A}(\mathbf{r})\). As a consequence of the \(\mathbf{r}\)-dependence of the vector potential, the \(x\) and \(y\) components of the new momenta become operators that no longer commute, \(\left[q_{x/y}, q_{x/y}\right] = -\mathrm{sgn}(v_x v_y)B/\lambda B\), in terms of the magnetic length \(\lambda B = 1/\sqrt{e|B|}\). In the following, we consider the tilt to have no component in the \(y\)-direction—this can always be achieved via a rotation and a possible rescaling of the momenta—and the Hamiltonian thus reads (see Supplemental Material [20])

\[
H_B = (\omega_\perp q_x + \omega_{0z} k_z) 1 + v_\perp (q_x \hat{\sigma}_x + q_y \hat{\sigma}_y) + v_z k_z \hat{\sigma}_z,
\]  

(3)

where \(v_\perp = \sqrt{|v_x v_y|}\) is the average Fermi velocity in the \(xy\)-plane, and \(\omega_\perp = v_\perp \sqrt{(\omega_{0x}/v_x)^2 + (\omega_{0y}/v_y)^2}\) is a rescaled tilt velocity.

While the Hamiltonian (3) can, in principle, within a lengthy calculation, be solved by the introduction of the usual ladder operators \(\hat{a}^\pm = \lambda B (q_x \pm i q_y)/\sqrt{2}\), similarly to the 2D case [21,22], a more elegant method consists of using a hyperbolic transformation to change the eigenvalue equation \((H_B - E 1)|\Psi\rangle = 0\) into

\[
(e^{i\theta/2} |\hat{\sigma}_x| H_B e^{i\theta/2}|\hat{\sigma}_x| - E |\hat{\sigma}_x|)|\tilde{\Psi}\rangle = 0,
\]  

(4)

where \(|\tilde{\Psi}\rangle = \mathcal{N} \exp(-\theta |\hat{\sigma}_x|/2)|\Psi\rangle\), and \(\mathcal{N}\) is a normalization constant required since the hyperbolic transformation does not preserve the norm of the wave functions. This transformation is nothing other than a Lorentz boost in the \(x\)-direction in terms of the relativistic parameter \(\tan\theta = |\beta|\) [8], which reads \(\beta = -\omega_\perp/v_\perp\) in the magnetic regime \((|\beta| < 1)\) and \(\beta = -v_\perp/\omega_\perp\) in the electric regime \((|\beta| > 1)\) [23]. As mentioned in the introduction, only the magnetic regime allows for quantized LLs, and we concentrate henceforth on this regime. In the transformed frame of reference, the eigenvalue equation (4) reads

\[
\gamma (\omega_{0z} \tilde{k}_z - E) 1 + v_\perp (\tilde{q}_x \hat{\sigma}_x + \tilde{q}_y \hat{\sigma}_y) + v_z k_z \hat{\sigma}_z |\tilde{\Psi}\rangle = 0,
\]  

(5)

where \(\gamma = (1 - \beta^2)^{-1/2}\) is the dilatation factor. The tilde indicates transformed wave vectors, \(\tilde{q}_x = q_x/\gamma + \gamma \beta (\omega_{0x} - E)/v_\perp\), \(\tilde{q}_y = q_y\), and \(\tilde{k}_z = k_z\), in agreement with a Lorentz boost in the \(x\)-direction [11].

One notices that the eigenvalue equation (5) now only contains the noncommutative wave vector components \(\tilde{q}_x\) and \(\tilde{q}_y\) in the off-diagonal matrix elements. It can therefore easily be solved by the introduction of the standard ladder operators, but with a renormalized \(B\) field because the commutation relations between the transformed wave vector components read \([\tilde{q}_x, \tilde{q}_y] = -\mathrm{sgn}(v_x v_y)B/\gamma \lambda B\) and \([\tilde{q}_x, k_z] = [\tilde{q}_y, k_z] = 0\). One thus finds the LLs

\[
E_{n,0}(k_z) = \alpha_0 k_z + \lambda \frac{1}{\gamma} \sqrt{v_\perp^2 k_z^2 + \frac{2 e B v_\perp^2}{\gamma} \lambda},
\]  

(6)

where \(\lambda = \pm 1\). Let us first discuss the different regimes. As mentioned above, LL quantization is only possible in the magnetic regime. Similarly to the tilt parameter (2), this can conveniently be described in terms of the in-plane tilt vector,

\[
\mathbf{t}_\perp = \mathbf{t} \times \mathbf{B} = \left(\frac{\omega_{0x}}{v_x}, \frac{\omega_{0y}}{v_y}\right).
\]  

(7)

Its norm is precisely \(|\beta|\) and can be related to the tilt parameter (2) and the angle \(\alpha\) between the magnetic field and the tilt direction, via \(|\beta| = |t_\perp| = |t||\sin \alpha|\). These geometric relations are shown in Fig. 1, where the sphere \(|t| = 1\) indicates the border between a type-I (inside) and a type-II WSM (outside). Similarly, the magnetic regime is represented by the inside (green) of the circle \(r_2^2 + r_1^2 = 1\) while the electric regime is situated outside. Whereas a type-I WSM, represented by the blue vector \(\mathbf{t}_{\text{m1}}\) inside the
sphere, has always a projection to the xy-plane inside the sphere, i.e., in the magnetic regime, one needs to distinguish two situations for type-II WSM. Below a critical angle $\alpha_c$, given by

$$|\sin \alpha_c| < 1/|t|,$$

the projection of the tilt vector ($t_{\theta z}$ in Fig. 1) is within the sphere and thus in the magnetic regime. However, if the condition (8) is not satisfied, the projection (of $t_{\theta z}$) is outside the unit circle, and the system is thus in the electric regime.

The LL spectrum (6) is represented in Fig. 2 for a type-I WSM [panel (a)] and a type-II WSM [panel (b)] in the magnetic regime. One retrieves the known 2D results for $k_z = 0$ [7,12,21], i.e., a graphenelike LL spectrum with $E_{n,\pm} \propto (1 - \beta^2)^{3/4} \sqrt{Bn}$, where the spacing is reduced by the relativistic factor $(1 - \beta^2)^{3/4}$. In the 3D case, these LLs evolve into one-dimensional (1D) bands with a dispersion in $k_z$. It is precisely this dispersion that gives information about the underlying WSM type since their bands are also tilted and can be seen as gapless ($n = 0$) or gapped ($n \neq 0$) Dirac cones with a tilt below (type-I) or above (type-II) the critical value. Their tilt is characterized by the 1D tilt parameter $t_z = \omega_0 / |v_z'|$, in terms of the velocity $v_z' = \sqrt{1 - \beta^2 v_z}$.

FIG. 2. LL spectrum of a tilted Weyl cone for $\beta = 0.75$, in units of $v_{\perp}/l_B = 26$ meV $\times v_{\perp} [10^6 \text{ m/s}] / \sqrt{B[T]}$. The green lines are $n = 0$ LLs and the blue (red) line represents the $n = 0$ state for $\text{sgn}(v_x, v_y, v_z) = 1$ [sgn$(v_x, v_y, v_z) = -1$]. The left figure corresponds to the case of a type-I Weyl semimetal where the $n = 0$ LL group velocity changes sign with chirality. On the contrary, the right figure is for a type-II Weyl semimetal, where the $n = 0$ slope representing the LL group velocity direction is independent of chirality.

$$t_z = \frac{|t| \cos(\alpha)}{\sqrt{1 - t^2 \sin(\alpha)^2}}.$$  (9)

One thus finds that for any angle $\alpha$ one has $t_z < 1$ for a type-I and $t_z > 1$ for a type-II WSM; i.e., the type of 1D band is the same as the original 3D WSM in the absence of a magnetic field.

A naturally arising question is whether one can also induce a transition from the magnetic to the electric regime in a type-I WSM. From a theoretical point of view, this can, in principle, be achieved by an electric field with a nonzero component perpendicular to $B$. Let us consider for simplicity an electric field $\mathbf{E}$ in the $y$-direction that yields a supplementary term $V = e\mathbf{E} \cdot \mathbf{y}^\dagger$ to Hamiltonian (1). In the Landau gauge $A = -Bye^\dagger$, the modified Hamiltonian reads $H_{A,B} = H_{B}^\dagger - (\mathbf{E}/B)k_z 1$, where $H_{B}^\dagger$ has the same structure as Eq. (3) if we replace the tilt velocity [9] $\omega_0 \to \omega = \omega_0 - \mathbf{E} \times \mathbf{B}/B^2$ or equivalently the tilt parameter $t \to t_z$, with

$$t_z = t - \frac{1}{B^2} \left[ \frac{\langle \mathbf{E} \times \mathbf{B} \rangle_x}{|v_x|} \frac{\langle \mathbf{E} \times \mathbf{B} \rangle_y}{|v_y|} \frac{\langle \mathbf{E} \times \mathbf{B} \rangle_z}{|v_z|} \right].$$  (10)

A type-I WSM can therefore undergo a transition from the magnetic to the electric regime for a judicious choice of the electric field if the criterion (8) is satisfied in terms of the tilt parameter $t_z$, inducing a breakdown of the LL spectrum [8,9]. From an experimental point of view, however, the situation is more involved because of the screening of the electric field due to free carriers both in the bulk and at the surfaces. Further studies are thus required to establish the feasibility of such experiments.

We show, however, that distinctive signatures of type-I and type-II WSM are clearly accessible in magneto-optical (reflectivity) experiments [24] in the magnetic regime, with no electric field involved. Within linear-response theory, the reflection of light at a polarization I is proportional to the real part of the optical conductivity,

$$\text{Re}\sigma_{\parallel\parallel}(\omega) = \frac{\sigma_0}{2\pi l_B^2 \omega} \sum_{j,j'} |\mathbf{V}_{jj'}|^2 \times [f(E_j) - f(E_{j'})] \delta(\omega - \omega_{jj'}),$$  (11)

where the subscripts $j$, $j'$ denote the quantum numbers $(\lambda, n, k_z)$, $\sigma_0 = e^2/2\pi$ is the quantum of conductance, and $\omega_{jj'} = E_j - E_{j'}$ is the energy difference between the final and initial states. Furthermore, $f(E_j)$ is the Fermi-Dirac distribution for a Fermi level that we choose at zero energy (at the position of the Weyl point) and the matrix element is given by $\mathbf{V}_{jj'} = \langle \Psi_{j'} | \nabla_k H_B | \Psi_j \rangle$. This formula is integrated analytically for two elliptic polarizations (see Supplemental Material [20]). One of the most salient features of the matrix elements in Eq. (11) is related to the nonorthogonality of the spinor components as a consequence of the relativistic boost.
interband peaks arise in the optical conductivity at energies

\[ \omega_{mn} = (1 - \beta^2)^{3/4} \sqrt{2eB} v_\perp (\sqrt{m + \sqrt{n}}). \] (12)

This is shown in Fig. 3 for a type-I [panel (a)] and a type-II WSM [panel (b)], where we depict the optical conductivity as a function of frequency for several values of \( \beta \). For \( \beta = 0 \), one retrieves the typical spectrum of a WSM discussed in the literature [25,26], where the peaks have the usual \( 1/\sqrt{\omega - \omega_{mn}} \) divergence due to the 1D character of the LL bands as a function of \( k_z \). These are also visible at \( \beta \neq 0 \) and are the main difference with respect to the 2D case discussed in Ref. [10]. Furthermore, the optical conductivity of an undoped type-II WSM shows additional peaks at low energies that are due to allowed transitions between LLs of the same original band. Indeed, LLs corresponding to the family \( \lambda = + \), which are always at positive energies in a type-I WSM, have parts of bands situated at negative energies, whereas those with \( \lambda = - \) become positive for certain values of \( k_z \). Therefore, transitions between LLs of the same family [red arrows in the inset of panel (a)] are no longer blocked by the Pauli principle and contribute to the optical conductivity up to the energy

\[ \omega_l = (1 - \beta^2)^{3/4} \sqrt{2eB} v_\perp \frac{\sqrt{2|t_z|}}{\sqrt{t_z^2 - 1}}. \] (13)

This yields the unusually large optical conductivity at low frequency and reflects the large density of states of a type-II WSM at zero \( B \) field, in comparison with a type-I WSM. The effect is different from that previously described in Ref. [25] for a type-I WSM where low-frequency peaks in the optical conductivity are obtained upon doping, whereas here the system is undoped.

In conclusion, we have shown that 3D WSM show a rich variety of phases in the presence of a magnetic field that unveil the underlying relativistic symmetry. In contrast to 2D systems, the magnetic and the electric regimes, with and without LL quantization, respectively, no longer coincide with the type of the WSM in 3D. Indeed, a type-II WSM can show LL quantization as long as the angle between the tilt direction and the magnetic field satisfies the condition (8)—in this case, the type-II character is visible in the 1D Landau bands as a function of the wave vector \( k_z \) in the direction of the \( B \) field. Most saliently, we have shown that the relativistic parameter \( \beta \) has a clear fingerprint in the optical conductivity, which can be probed in magneto-optical measurements, discerning different types of WSM. We finally emphasize that our results are readily generalized to the case of a pair (or more) of Weyl points in a more realistic band structure. If the two cones are related by a discrete symmetry (e.g., time reversal), the tilts of the two cones are in opposite directions. In this case, one obtains two copies of the same LL spectrum, since the parameter \( \beta \) depends only on the modulus of the tilt vector \( t_\perp \). For more pairs of Weyl points, the tilt vectors are no longer necessarily of the same modulus, and the condition (8) for the transition between the magnetic and electric regime is then not unique for all points. Recently, we became aware of two other preprints on magnetic-field properties of type-II WSM. The findings of Ref. [27] are similar to ours but the authors consider only the optical conductivity for \( \beta = 0 \), i.e., when the tilt is in the same direction as the \( B \) field, in which case one has no violation of the dipolar selection rule \( n \to (n \pm 1) \) and no renormalization of the LL spacing. The authors of Ref. [28] study the chiral
anomaly furthermore in a lattice tight-binding model and extract numerically the optical conductivity of a type-II WSM in the magnetic regime.

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