Chiral filtration of light by Weyl-semimetal medium

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Recently discussed topological materials Weyl-semimetals (WSs) combine both: high electron mobility comparable with graphene and unique topological protection of Dirac points. We present novel results related to electromagnetic field propagation through WSs. It is predicted that transmission of the normally incident polarized electromagnetic wave (EMW) through the WS strongly depends on the orientation of polarization with respect to a gyration vector \mathbf{g} . The latter is related to the vector-parameter \mathbf{b} , which represents the separation between the Weyl nodes of opposite chirality in the first Brillouin zone. By changing the polarization of the incident EMW with respect to the gyration vector \mathbf{g} the system undergoes the transition from the isotropic dielectric to the medium with Kerr- or Faraday-like rotation of polarization and finally to the system with chiral selective electromagnetic field. It is shown that WSs can be applied as the polarization filters.

The experimental discovery of the 3D Dirac fermions in Na₃Bi and Cd₃As₂ [1–3] has opened a new window of possibilities in condensed matter and material science with Weyl semimetals (WSs) [4–9]. These materials are characterized by broken time-reversal or inversion symmetry. The Brillouin zone of a WS contains pairs of Weyl nodes. Since these nodes can become sources and sinks of Berry curvature, unusual surface states can be formed [10]. WS can be viewed as a 3D generalization of graphene, where the Dirac points are not gapped by the spin-orbit interaction, and the crossing of the linear dispersions is protected by crystal symmetry [11]. The Dirac nature of the quasiparticles in WS was confirmed by investigating the electronic structure of these materials with angle-resolved photoemission spectroscopy and a very high electron mobility was observed, up to 2.8×10^5 cm²/Vs [1–3], which is comparable to that of the best graphene. The magnetotransport in Dirac materials was studied in Ref. [12]. The optical conductivity tensor of a 3D Weyl semimetal was evaluated from semiclassical Boltzmann transport theory [13]. Nontrivial topology of WS manifests itself in the interesting optical properties [14, 15]. A new way to isolate real topological signatures of bulk states in WSs was developed [16]. Properties of WSs are reviewed in Ref. [17, 18].

In this letter we investigate the interplay between the topological nature of WSs and their optical properties. It is predicted that WS can behave as broadband chiral optical medium that selectively transmits and reflects circularly polarized electromagnetic field in wide range of frequencies. The search for a chiral optical medium has been marked by the discovery of liquid crystals having chiral selective transmission and reflection [19]. Later photonic crystals and metamaterials with similar properties, but in a narrower frequency range, have been manufactured [20]. In this paper we predict that topologically nontrivial solid state crystals - Weyl semimetals may behave like a chiral optical medium.

In WSs the valence and conduction bands touch each other at the isolated points of the Brillouin zone, termed as Weyl nodes, close to the energy level of the chemical potential μ . The Hamiltonian \hat{H} of the charge carriers in the momentum space near a Weyl node is given by $\hat{H} = \chi v_F \mathbf{p} \cdot \hat{\sigma} - \mu$ [21, 22], where $\chi = \pm 1$ is the chirality, v_F is the Fermi velocity, \mathbf{p} is the momentum, and $\hat{\sigma}$ represents Pauli matrices. A doped Weyl semimetal with a positive chemical potential $\mu > 0$ is under consideration in this paper.

Weyl nodes of WS form pairs of opposite chirality [23–25]. Let us consider a WS with two Weyl nodes, which are separated in the first Brillouin zone by the wave vector **b**. Then the electromagnetic term of WS action acquires the topological θ -term $S_{\theta} = \frac{e^2}{4\pi\hbar} \int dt \int d^3r \, \theta \mathbf{E} \cdot \mathbf{B}$ [26–29]. In the latter expression e is the electron charge, **r** is the coordinate vector, t is time, $\chi = \pm 1$ and $\theta = 2 (\mathbf{b} \cdot \mathbf{r} - b_0 t)$. If $\theta = 0$ the system is not characterized by the topological properties.

The θ -term in the action results in the appearance of two nontrivial terms in the relation between the displacement field **D** and the electric field **E** in WS [13, 30–37]:

$$\mathbf{D} = \varepsilon_0(\omega)\mathbf{E} + \frac{e^2}{\pi\hbar\omega}(\nabla\theta) \times \mathbf{E} + \frac{ie^2}{\pi\hbar\omega}\dot{\theta}\mathbf{B},\tag{1}$$

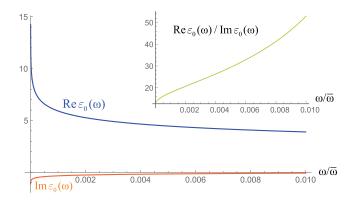


FIG. 1: (Color online) For chosen parameters, $\varepsilon_0'(\omega) \gg |\varepsilon_0''(\omega)|$. Thus, the attenuation of electromagnetic waves due to $|\varepsilon_0''| \neq 0$ is weak.

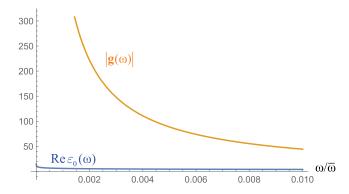


FIG. 2: (Color online) Comparison of the first and second terms of the dielectric tensor of a WS.

where the last two term present the anisotropy in the dielectric tensor. The the isotropic term $\varepsilon_0(\omega)$ in the dielectric tensor is related to the Coulomb interaction between electrons. At zero temperature in the framework of a tight-binding model with a strong spin-orbit interaction in Ref. [37] the complex dielectric constant for 3D semimetals was calculated as $\varepsilon_0(\omega) = \varepsilon'(\omega) + i\varepsilon''(\omega)$ with

$$\varepsilon'(\omega) = 1 + A \ln \left(\frac{B}{\omega}\right) \left[1 + F \ln \left(\frac{B}{\omega}\right)\right],$$

$$\varepsilon''(\omega) = D \left[1 + \alpha \left(E \ln \left(\frac{\omega}{\omega}\right) + C\right)\right],$$
(2)

when the ultraviolet cutoff frequency $\bar{\omega} \gg \omega$. In Eqs. (2) $A = \frac{N_W e^2}{3\pi v_F \hbar}$, where $N_W = 2$ is the number of Weyl points, $v_F = 10^6$ m/s, $B = \Lambda v_F$, where $\Lambda = \frac{\pi}{a_0}$ is the UV cutoff and $a_0 = 3$ Å is the length of a lattice vector, $C = -\frac{5}{3\pi}$, $D = \frac{N_W e^2}{6v_F \hbar}$, $E = \frac{2}{3\pi}$, $F = \frac{\alpha}{3\pi}$, and $\alpha = \frac{e^2}{\epsilon_W v_F \hbar}$, where $\epsilon_W = 3$ is the intrinsic dielectric constant.

The ultraviolet cutoff frequency $\bar{\omega}$ can be defined from the following expression for the density of electronic states, which equals the atomic concentration n in the tight-binding model:

$$n = 2 \int \frac{d^3 p}{(2\pi\hbar)^3} = \frac{1}{\pi^2 \hbar^3} \int_0^{\hbar\bar{\omega}} \frac{\mathcal{E}^2}{v_F^3} d\mathcal{E} = \frac{(\bar{\omega})^3}{3\pi^2 v_F^3} , \qquad (3)$$

where the factor of 2 in front of the integral stands for two valleys, and $\mathcal{E} = v_F p$ is the Dirac energy spectrum of the electrons in WSs. In our calculations we scaled the frequency in units of $\bar{\omega} = \sqrt[3]{3\pi^2 nc} v_F$ as the energy (frequency) unit in all figures. For material parameters given above, $\bar{\omega} \approx 2\pi \times 1.6 \times 10^{15}$ Hz.

In fact for given parameters $\varepsilon_0'(\omega) \gg |\varepsilon_0''(\omega)|$, as it is seen in Fig. 1. Thus, the attenuation of electromagnetic waves (EMWs) due to $\varepsilon_0'' \neq 0$ is weak.

As it follows from Eq. (1) (see Supplementary material A, the dielectric tensor of a WS can be written as

$$\varepsilon_{\alpha\beta}(\omega) = \varepsilon_0(\omega)\delta_{\alpha\beta} + i\epsilon_{\alpha\beta\gamma}g_{\gamma}(\omega). \tag{4}$$

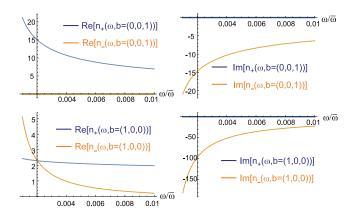


FIG. 3: (Color online) Refraction coefficients at different orientations of **b**. Since $|\operatorname{Im} N_{-}| \gg 1$, electromagnetic waves in z-direction with "-" chirality can not propagate.

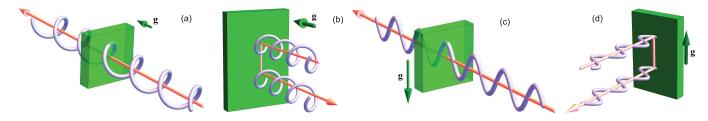


FIG. 4: (Color online) The figure schematically shows the filtering of light by polarization by the Weyl semimetal depending on the direction of the gyration vector \mathbf{g} (shown by green arrows). In (a) and (b) \mathbf{g} and \mathbf{k} are parallel. Then EMWs (a) transmit through WS for one chirality (type of circular polarization); (b) reflect for the other chirality (opposite circular polarization). In (c) and (d) \mathbf{g} and \mathbf{k} are perpendicular. Then EMWs (c) transmit for collinear with \mathbf{g} linear polarization and (d) reflect otherwise.

In Eq. (4) $\epsilon_{\alpha\beta\gamma}$, where $\alpha\beta\gamma$ corresponds xyz, is the fully antisymmetric tensor, $g_{\gamma}=-a(\omega)b_{\gamma}$ is the gyration vector [38] and $a(\omega)=\frac{2e^2}{\pi\hbar\omega}$ is an odd real function of ω , $a(\omega)=-a(-\omega)$. The second term in the dielectric tensor (4) is the Hermitian matrix and so it does not produce any dissipation despite the fact that it is purely imaginary.

The dielectric tensor (4) is well known in magnetooptics [38], where the gyration vector \mathbf{g} is typically ω independent and it is generally small compared to ε_0 (to first order, \mathbf{g} is proportional to the applied magnetic field, it is small, and it is considered as a "relativistic effect"). In contrast, for a WS the situation is opposite: $|\mathbf{g}| \sim |\varepsilon_0|$ (see Fig. 2), \mathbf{g} is essentially ω -dependent and the direction of \mathbf{g} is defined by the "built in" into WS material vector \mathbf{b} related to the Weil points.

We can estimate the amplitude of the second antisymmetric term in the dielectric tensor: $g(\omega) = a(\omega)b = \frac{2e^2b}{\pi\hbar\omega} = \frac{e^2}{\hbar c} \frac{2c\Lambda}{\pi\bar{\omega}} (b/\Lambda) \frac{\bar{\omega}}{\omega} \approx 1.45 (b/\Lambda) \frac{\bar{\omega}}{\omega}$. Typically $\omega \ll \bar{\omega}$ while $b/\Lambda \sim 1$, so $a(\omega)b \gg 1$. This is illustrated in Fig. 2. Note that we neglect surface induced contribution to the reflection coefficient because the contribution to the

Note that we neglect surface induced contribution to the reflection coefficient because the contribution to the reflection coefficient from the surface is much less than the contribution from the bulk [15].

We consider a monochromatic EMW in the WS medium with the dielectric tensor (4). Then for the electric field

$$\mathbf{E} = A\mathbf{p} \exp(i\mathbf{k} \cdot \mathbf{r} - i\omega t),\tag{5}$$

where A is the amplitude, **p** is the unit vector fixing the wave polarization, we introduce the vector $\mathbf{n} = c\mathbf{k}/\omega$. The absolute value of $n = |\mathbf{n}|$ is usually treated as the refraction coefficient for the wave. From the Maxwell equations it follows that

$$(n^2\delta_{ik} - n_i n_k - \varepsilon_{ik})E_k = 0. (6)$$

This condition known as Fresnel equation allows to find \mathbf{p} and \mathbf{n} for a given direction of the wave. Assuming that the EMW goes along the z-direction and using expressions for ε_{ik} from Supplementary material A (see Eq. (S4)), one

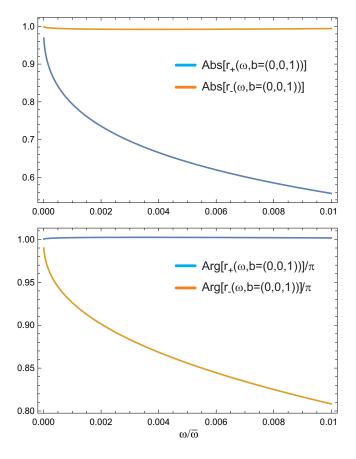


FIG. 5: (Color online) Reflection coefficients from the Weyl-semimetal half-space (z > 0) when b = (0, 0, 1).

can conclude that Eq. (6) has non-trivial solutions only if the following condition holds:

$$\det \begin{vmatrix} n^2 - \varepsilon_0 & ig_z & -ig_y \\ -ig_z & n^2 - \varepsilon_0 & ig_x \\ ig_y & -ig_x & -\varepsilon_0 \end{vmatrix} = 0.$$
 (7)

Eq. (7) can be reduced to the quadratic equation for n^2 , presented in Supplementary material B, which has two solutions labeled by $\sigma = \pm$:

$$n_{\sigma}^{2} = \varepsilon_{0} - \frac{g_{x}^{2} + g_{y}^{2} \mp \sqrt{(g_{x}^{2} + g_{y}^{2})^{2} + 4\varepsilon_{0}^{2}g_{z}^{2}}}{2\varepsilon_{0}}.$$
(8)

Let us analyze the solution (8) for the different polarization of the EMW and consider two limiting cases. First we consider $\mathbf{g} = (0, 0, g)$. Then

$$n_{\sigma}^2 = \varepsilon_0 \pm g, \qquad \mathbf{p}_{\sigma} = \begin{pmatrix} \pm i \\ 1 \\ 0 \end{pmatrix}.$$
 (9)

That solution formally describes two circularly polarized plane waves.

If $\mathbf{g} = (g_x, g_y, 0)$ then

$$n_+^2 = \varepsilon_0, \qquad n_-^2 = \varepsilon_0 - \frac{g_x^2 + g_y^2}{\varepsilon_0}, \tag{10}$$

and

$$\mathbf{p}_{+} \propto \begin{pmatrix} g_{x} \\ g_{y} \\ 0 \end{pmatrix}, \qquad \mathbf{p}_{-} \propto \begin{pmatrix} ig_{y}\varepsilon_{0} \\ -ig_{x}\varepsilon_{0} \\ g_{x}^{2} + g_{y}^{2} \end{pmatrix}. \tag{11}$$

Now we investigate reflection of EMW from the WS interface when the **k** vector is perpendicular to the interface. WS occupies z > 0 half-space, while the left-half space z < 0 is an isotropic dielectric with susceptibility ε_d . Then the electric field is given by

$$\mathbf{E} = \mathbf{p}_d \left(e^{i\omega n_d z/c - i\omega t} - r e^{-i\omega n_d z/c - i\omega t} \right), \quad z < 0,$$

$$\mathbf{E} = A \mathbf{p} e^{i\omega n z/c - i\omega t}, \quad z > 0,$$
(12)

where $n_d = \sqrt{\varepsilon_d}$, **p** and *n* here is either **p**₊ (n_+) or **p**₋ (n_-) and *r* is the reflection coefficient. The magnetic field of this EMW can be presented as

$$\mathbf{B} = \mathbf{q}_d \times \mathbf{p}_d \left(e^{i\omega n_d z/c - i\omega t} + r e^{-i\omega n_d z/c - i\omega t} \right), z < 0,$$

$$\mathbf{B} = A\mathbf{q} \times \mathbf{p} e^{i\omega n z/c - i\omega t}, \qquad z > 0,$$
(13)

where $\mathbf{q}_d = (0, 0, n_d/c)$ and $\mathbf{q} = (0, 0, n/c)$ and for simplicity we again omit the index $\sigma = \pm$).

One can choose an arbitrary polarization vector of the incident wave in the dielectric, \mathbf{p}_d , perpendicular to z-direction. But we choose the specific \mathbf{p}_d — collinear to the transverse components of polarization vector \mathbf{p} in WS:

$$\mathbf{p}_d = (p_x, p_y, 0) / \sqrt{p_x^2 + p_y^2},\tag{14}$$

so $\mathbf{p}_d \times \mathbf{p} = 0$.

Transverse components of electric field and magnetic field are continuous at the interface. Then from Eqs. (12)-(13) it follows,

$$1 - r = A\sqrt{p_x^2 + p_y^2}, \quad n_d(1+r) = nA\sqrt{p_x^2 + p_y^2}, \tag{15}$$

and we get the reflection coefficient

$$r_{\sigma} = \frac{n_d - n_{\sigma}}{n_d + n_{\sigma}}. (16)$$

Here we restored the σ -index. One should pay attention that the simple expression (16) for r_{σ} is correct only for very specific choice of incident wave polarization in the dielectric half-space.

First we consider the case when the gyration vector (or **b**) is parallel to the **k** vector of the EMW. Then only circular polarized EMW with polarization $\mathbf{p} = (i, 1, 0)$ can propagate through WS. As it follows from Eq. (9), $n_-^2 < 0$ for $g = g_z > \varepsilon'_0$. Taking the circular polarized wave with polarization $\mathbf{p} = (-i, 1, 0)$ as the incident wave on WS surface we get from Eq. (16), $|r_-| = 1$ which means full reflection. The wave with polarization $\mathbf{p} = (i, 1, 0)$ have finite probability of transmission through WS interface, see Fig. 5. So WS can serve as the polarization filter that filters from the incident electromagnetic irradiation circular polarized EMWs with certain polarization. The direction of the electric field of a circular polarized light forms a spiral in space. If the spiral twist in the direction of \mathbf{g} satisfies "the right hand rule" (clockwise) then this radiation can go through WS, as it is shown in Fig. 4a.

Certain chirality ± 1 can be attributed to circular polarization depending on its "right-hand" or "left-hand" nature (wether the helix describes the thread of a right-hand or left-hand screw, respectively). So WS — the host of chiral electrons is also the system with chiral selectively of electromagnetic field, see Fig. 4a and b.

Now we consider the case when $\mathbf{b} \perp \mathbf{k}$. Then only linear polarized EMW with $\mathbf{p} = \mathbf{p}_+ = (b_x, b_y, 0)$, see Eq. (11), can propagate through WS. The wave with the orthogonal polarization $\mathbf{p}_- = (-b_x, b_y, 0)$ fades out if $\varepsilon_0 < \sqrt{g_x^2 + g_y^2}$, see Eq. (10). Thus, in this case WS can serve as the polarization filter that filters from the incident electromagnetic irradiation linearly polarized EMWs along \mathbf{b} .

In the intermediate case, when there is a certain nonzero angle between **b** and **k** (different from $\pi/2$), WS filters certain elliptic polarized waves.

Conclusions. In this Letter we have obtained the frequency dependencies of the refraction and reflection coefficients for the Weyl semimetal for the different orientations of the vector **b**, which denotes the separation between the Weyl nodes of opposite chirality in the first Brillouin zone and defines the gyration vector **g**. It is predicted that the propagation of the normally incident polarized electromagnetic wave through the WS for each polarization strongly depends on the orientation of the polarization with respect to the gyration vector **g**: when the normally incident electromagnetic wave is collinear to the gyration vector it is transmitted through the WS for one circular polarization,

while it is reflected for the opposite circular polarization; the normally incident electromagnetic wave with the linear polarization is transmitted through the WS if the polarization is collinear to the gyration vector and reflected if the polarization is normal to the gyration vector. The results of calculations demonstrated that via changing the polarization of the normally incident electromagnetic wave with respect to the vector **b** the WS changes its behavior from the isotropic dielectric to the medium with Kerr- or Faraday-like rotation of polarization and also to the system with chiral selective electromagnetic field. We propose that WSs can be applied as the polarization filters.

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