High-order harmonic generation in three-dimensional Weyl semimetals

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In this paper, the nonlinear interaction of Weyl semimetal (WSM) with a strong driving electromagnetic wave-field is investigated. In the scope of the structure-gauge invariant low-energy nonlinear electrodynamics theory, the polarization-resolved high-order harmonic generation spectra in WSM are analyzed. The obtained results show that the spectra in WSM are completely different compared to 2D graphene case. In particular, at the non-collinear arrangement of the electric and Weyl nodes’ momentum separation vectors, an anomalous harmonics are generated which are polarised perpendicular to the pump wave electric field. The intensities of anomalous harmonics are quadratically dependent on the momentum space separation of the Weyl nodes. If the right and the left Weyl fermions are merged, we have a 4-component trivial massless Dirac fermion and, as a consequence, the anomalous harmonics vanish. In contrast to the anomalous harmonics, the intensities of normal harmonics do not depend on the Weyl nodes’ momentum separation vector, and the harmonics spectra resemble the picture for a massless 3D Dirac fermion.

I. INTRODUCTION

As a three-dimensional analogs of graphene [11, 12], the Dirac semimetals (DSM) [3–6] and the WSM [7,12] have been implemented in a variety of condensed matter systems. These materials are three-dimensional quantum phases of the matter with gapless electronic excitations that are protected by topology and symmetry [13]. The low energy dispersion of such materials contains conical intersections and diabolical points, which are referred to as a Dirac points, or a Weyl nodes [14]. The DSMs possess both time-reversal and spatial inversion symmetry. When one of these symmetries is broken, the Dirac points are split into the pair of the Weyl nodes, and the medium becomes a WSM. The low energy theory of the simplest WSM is described by the Weyl Hamiltonian [15] near the Weyl nodes where the right-handed and the left-handed chirality fermions are separated in the momentum space. Due to the nontrivial topology of the bands, the Berry curvature in the momentum space is nonzero [16, 17], and we have an appropriate case of the Dirac monopole/antimonopole [18] realization in the momentum space [19]. As a result, the linear electromagnetic (EM) response of the three-dimensional WSM is described by an axionic field theory [20, 22] with the anomalous linear electrodynamics effects [23–27]. The interaction between the strong EM waves and WSM gives rise to nonlinear optical effects, such as the photovoltaic effect [28, 29], optical rectification and second-harmonic generation [30, 32], terahertz emission [33] and third harmonic generation [34]. These are perturbative nonlinear optical effects. With the further increase of the driving wave intensity, the extreme nonlinear optical effects [35] may be visible in pseudo-relativistic systems. In particular, the high-order harmonic generation (HHG) is an essential nonlinear dynamic process that can be used as a probe to extract the properties of a medium. It can also be useful for new nanodevices. To date, HHG has been observed in graphene [36], in DSM [37, 38], in topological insulators [39], and in WSM [40], where the “spike-like” Berry curvature may generate even-order harmonics. Note that as in graphene, there is quite a high carrier mobility in WSM [41, 42], that is the electrons can move significantly in the Brillouin zone, which is favorable for HHG phenomenon in nanostructures.

As is well studied for graphene the HHG process at Dirac-cone approximation [13–14] significantly different from the HHG when electrons can move significantly in the Brillouin zone, here polarization and optical anisotropy effects of HHG in graphene arise [49–57]. The HHG in WSM with particular lattice realization theoretically is studied in Ref. [58] where anisotropic anomalous HHG from time-reversal symmetry broken WSM is reported. Nonperturbative topological intraband current in WSM and DSM in laser fields has been investigated in Ref. [59] for general case, without lattice concretization. To establish a nonlinear response intrinsically connected to topology one should arise from the universal Weyl Hamiltonian which is the root of the field theory anomalies. Hence, there is tremendous interest from the strong fields physics perspectives in understanding how the field theory anomalies affect the nonlinear response of WSM at low energy excitations where the theory is universal and does not depend on the particular lattice realization of the WSM. To this end, in the current paper we investigate the low-energy nonlinear electrodynamics of WSM and analyze polarization-resolved high-order harmonic generation spectra in WSM. The consideration is based on structure-gauge invariant low-energy nonlinear electrodynamics where an ansatz applied to the Dirac monopole [60] is adopted to overcome the topological singularity.

The paper is organized as follows. In Sec. II the structure-gauge invariant low-energy nonlinear electrodynamics theory with evolutionary equation for the single-particle density matrix is presented. In Sec. III, we consider polarization-resolved HHG spectra and present the main results. Finally, conclusions are given in Sec. IV.

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II. MODEL HAMILTONIAN AND THE EVOLUTIONARY EQUATION FOR THE SINGLE-PARTICLE DENSITY MATRIX

We will start from the low energy universal Hamiltonian involving 4-component massless Dirac fermion:

$$\hat{H}_0 = v \int d^3x \hat{\Psi} \left[ -i\gamma^j \partial_j + b_\mu \gamma^\mu \gamma^5 \right] \hat{\Psi}$$  \hspace{1cm} (1)

where $v$ is the Fermi velocity, $\hat{\Psi} = \Psi^\dagger \gamma_0$, matrices $\gamma^0$ and $\gamma^j$ ($j=1,2,3$) are Dirac anticommuting $\gamma$ matrices, $\gamma^5 = i\gamma^0 \gamma^1 \gamma^2 \gamma^3$ is the chirality matrix, and $b_\mu$ is the axial 4-vector. In the chiral representation of the $\gamma$ matrices we have

$$\gamma^0 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \gamma = \begin{pmatrix} 0 & \sigma \\ -\sigma & 0 \end{pmatrix}, \quad \gamma^5 = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix},$$

(2)

where $\sigma$ is the vector operator formed out of three Pauli matrices. In Eq. (1) the term proportional to $b_\mu$ breaks $CPT$ symmetry. In this paper we will consider the case of space-like axial vector $b_0 = 0$. In this case axial vector term $b_\mu \gamma^\mu$ preserves inversion ($P$) and charge conjugation ($C$) symmetries, but breaks time reversal symmetry ($T$). Note that this case is more feasible for the realization of a Weyl semi-metal and the corresponding minimal lattice model can easily be constructed [27]. The Hamiltonian $\hat{H}_0(k)$ in the momentum space becomes

$$\hat{H}_0(k) = v \left( \sigma \cdot (k + b) \right) : \chi = \pm 1.$$  \hspace{1cm} (3)

For compactness of equations atomic units are used throughout the paper unless otherwise indicated. The eigenstates of this Hamiltonian are also eigenstates of chirality matrix $\gamma^5$ with eigenvalues $\chi = \pm 1$. Since Dirac mass is zero, the $\hat{H}_0(k)$ is block diagonal and the left-handed $(1 - \gamma^5) \Psi/2$ and right-handed components $(1 + \gamma^5) \Psi/2$ of the Dirac field are decoupled to left-handed and right-handed two-component Weyl spinors, described by the Hamiltonians

$$\hat{H}_\chi = -\chi \sigma \cdot (k - \chi b) \chi = \pm 1.$$  \hspace{1cm} (4)

The $2 \times 2$ Hamiltonians $\hat{H}_1$ and $\hat{H}_{-1}$ also describe the monopole and the anti-monopole of the Berry curvature in the momentum space, respectively [17,69]. For $b \neq 0$, the right and the left Weyl fermions are separated in the momentum space and the WSM is topologically non-trivial. The eigenvalues $\chi = \pm 1$ also have topological notion. The Berry flux piercing any surface enclosing the Weyl nodes $k_\chi b$ is exactly $2\pi\chi$, i.e. $\chi$ also defines the Chern number or topological charge. In accordance with Nielsen-Ninomiya theorem the Weyl nodes should come in opposite chirality pairs [31]. When $b = 0$ these Weyl nodes are merged giving rise to topologically trivial, 4-component massless Dirac fermion.

For the calculation of the nonlinear EM response of WSM we need eigenstates of the Hamiltonian [4]. With these eigenstates we should calculate Berry connection and then curvature. Because of the monopole in momentum space, the eigenstates of the Weyl Hamiltonian (1) cannot be defined globally for all $k$. The eigenstates $|\beta, \chi, k\rangle$, where $\chi$ refers to band index, can be subject to an arbitrary structure-gauge [62] transformation

$$|\beta, \chi, k\rangle' = e^{i\tilde{\alpha}(\chi,k)|\beta, \chi, k\rangle}$$

(5)

without changing the physical properties of the system. For the quantum kinetics we need to calculate the transition dipole moments $d_{\beta\beta'}(\chi, k) = \langle \beta, \chi, k | i\partial_b | \beta', \chi, k \rangle$. The Berry connections are defined as the diagonal elements $A_{\beta}(\chi, k) = d_{\beta\beta}(\chi, k)$. Hence, due to the gradient $\partial_b$ a smooth structure gauge for the eigenstates is thus required. To overcome this problem we will adopt the ansatz applied to Dirac monopole. To this end we choose axial vector $b$ directed along the x-axis $b = b\hat{x}$ and define the eigenstates for $k_z \geq 0$ for $k_z \leq 0$ we have

$$|c, \chi, k\rangle_+ = \frac{1}{\sqrt{2k^2 + 2k_xk_z}} \left[ \frac{k_x + k_z}{k_x + ik_y} \right],$$

(6)

$$|v, \chi, k\rangle_+ = \frac{1}{\sqrt{2k^2 + 2k_xk_z}} \left[ \frac{-k_x + ik_y}{k_x + k_z} \right],$$

(7)

for $k_z \leq 0$ we have

$$|c, \chi, k\rangle_- = \frac{1}{\sqrt{2k^2 + 2k_xk_z}} \left[ \frac{k_x - ik_y}{k_x - k_z} \right],$$

(8)

$$|v, \chi, k\rangle_- = \frac{1}{\sqrt{2k^2 + 2k_xk_z}} \left[ \frac{-k_x + k_z}{k_x + ik_y} \right],$$

(9)

where $k_x = x - \chi b$ and $k_x = \sqrt{k_x^2 + k_y^2 + k_z^2}$. The eigenenergies are: $E_{c\chi}(k) = vk_x$ and $E_{v\chi}(k) = -vk_x$.

The solutions for the opposite chirality are: $|c, \chi, k\rangle_\pm = |c, \chi, -k\rangle_\mp$ and $|v, \chi, k\rangle_\pm = |v, \chi, -k\rangle_\mp$. At the overlap $k_z = 0$ solutions [6], [8], and [7], [9] are connected by the gauge transformation:

$$\langle c, \chi, k | = e^{i\tilde{\alpha}(k_x, k_y)} | c, \chi, k\rangle_+,$n

$$|v, \chi, k| = e^{-i\tilde{\alpha}(k_x, k_y)} | v, \chi, k\rangle_+,$

where $\tilde{\alpha}(k_x, k_y) = \arctan(k_y/k_x)$. From Eqs. [6], [8], [7], and [9] for the total Berry connection $A(\chi, k) = \langle c, \chi, k | i\partial_b | c, \chi, k\rangle - \langle v, \chi, k | i\partial_b | v, \chi, k\rangle$ we obtain:

$$A_+ (\chi, k) = -\chi \frac{k_y \hat{x} - k_x \hat{y}}{k_x^2 + k_y^2}.$$  \hspace{1cm} (10)
For the Berry curvature $\mathcal{B}(\chi, k) = \partial A^\chi \times A(\chi, k)$ we obtain located at the Weyl node $k = \chi b$ monopole field

$$B_x = e k_x k^\chi, \quad B_y = e k_y k^\chi, \quad B_z = e k_z k^\chi,$$

with $\text{div} \mathcal{B} = 4\pi \delta (k - \chi b)$ and $\delta$ is the Dirac delta function. For the transition dipole moments we have

$$d_{\epsilon v+} (\chi, k) = \left( ik x - \chi k y \right) \tilde{z} + \frac{1}{2k^2} \left( k^x k_y - k^2 \right) + 
\begin{aligned}
&
\left( i \left( k^2 - k^x - k^y \right) \right) \tilde{x} \\
+&
\left( \chi \left( k^x + k^y - k^2 \right) + i k^x k^y \right) \tilde{y}.
\end{aligned}$$

(13)

$$d_{\epsilon v-} (\chi, k) = \left( ik x + \chi k y \right) \tilde{z} - \frac{1}{2k^2} \left( k^x k_y - k^2 \right) - 
\begin{aligned}
&
\left( \chi \left( k^x - k^y - k^2 \right) - i k^x k^y \right) \tilde{y}.
\end{aligned}$$

(14)

Note the following useful relations

$$\frac{1}{2} \epsilon^{abc} \mathcal{B}^c (\chi, k)$$

$$= i \left\{ d_{\epsilon v}^a (\chi, k) d_{\epsilon v}^b (\chi, k) - d_{\epsilon v}^b (\chi, k) d_{\epsilon v}^a (\chi, k) \right\},$$

(15)

where $\epsilon^{abc}$ is the Levi-Civita symbol and the summation over the repeated upper indices is implied. This equation is gauge invariant and connects the transition dipole moments with the Berry curvature. Here for the sake of brevity, we omit the indices ($\pm$).

The semiconductor Bloch equations (SBEs) governing a WSM driven by a strong laser field in the length gauge read:

$$\partial_t \rho_{\alpha \beta;\chi} (k_0, t) = i \mathcal{E}_{\alpha \beta;\chi} (k_0 + A) \rho_{\alpha \beta;\chi} (k_0, t)$$

$$- (1 - \delta_{\alpha \beta}) \Gamma \rho_{\alpha \beta;\chi} (k_0, t) + i \sum_{\alpha'} d_{\alpha' \beta} (\chi, k_0 + A) \rho_{\alpha \alpha';\chi} (k_0, t),$$

(16)

where $\rho_{\alpha \beta;\chi}$ are the single particle density matrix elements, $E$ is the laser electric field strength, $A = - \int_0^t E (t') dt'$ is the vector potential, $\mathcal{E}_{\alpha \beta;\chi} (k) = \mathcal{E}_{\beta;\chi} (k) - \mathcal{E}_{\alpha;\chi} (k)$, and $\Gamma$ is the dephasing time. The crystal momentum $k$ has been transformed into a frame moving with the vector potential $k_0 = k - A$. Note that in Eq. (16), the Berry connections $[10]$ and $[11]$ are included $d_{\alpha \beta} (\chi, k) = A_{\beta} (\chi, k)$.

The optical excitation induces a volume current that can be calculated by the following formula:

$$\mathbf{j} (t) = - \left[ \sum_{\alpha \chi k_0} \left( V_{\alpha \chi} (k_0 + A) \right) \rho_{\alpha \chi;\chi} (k_0, t) \right]$$

$$+ i \sum_{\alpha \chi k_0} \sum_{k_0} d_{\alpha} (\chi, k_0 + A) \mathcal{E}_{\beta;\chi} (k_0 + A) \rho_{\alpha \beta;\chi} (k_0, t),$$

(17)

where the band velocity is defined by $V_{\alpha \chi} (k) = \partial_{\chi} \mathcal{E}_{\alpha;\chi} (k)$. Note that Eqs. (16) and (17) provide structure-gauge invariant kinetic theory. Thus, at the structure-gauge transformation $[5]$ we have

$$d'_{\alpha \beta} (\chi, k) = e^{i \theta_{\alpha \beta} (k) - i \theta_{\alpha \beta} (k)} d_{\alpha \beta} (\chi, k),$$

$$\mathcal{A}'_{\alpha} (\chi, k) = \mathcal{A}_{\alpha} (\chi, k) - \partial_{\chi} \theta_{\alpha;\chi} (k),$$

$$\mathcal{B}' (\chi; k) = \mathcal{B} (\chi; k),$$

$$\rho'_{\alpha \beta;\chi} (k_0, t) = e^{i \theta_{\alpha \beta} (k_0 + A) - i \theta_{\alpha \beta} (k_0 + A)} \rho_{\alpha \beta;\chi} (k_0, t),$$

$$\mathbf{j}' (t) = \mathbf{j} (t).$$

III. RESULTS

We explore the nonlinear response of a WSM in a laser field of ultrashort duration:

$$E (t) = f (t) E_0 \hat{e} \cos (\omega t),$$

(18)

where $f (t) = \sin^2 (\pi t / \tau)$ is the sin-squared envelope function, $\tau$ is the pulse duration, $\hat{e}$ is the unit polarization vector, $\omega$ is the carrier frequency, $E_0$ is the electric field amplitude. We take a ten-cycle fundamental laser field.

As in graphene, the wave-particle interaction in WSM is characterized by the dimensionless parameter $[44]$

$$\xi_0 = \frac{e E_0 v}{\omega h \omega},$$

(19)

which represents the work of the wave electric field $E_0$ on a period $1 / \omega$ in the units of photon energy $h \omega$. The
parameter is written here in general units for clarity. For two band WSM system SBEs (16) are reduced to a closed set of equations for the interband polarization $P_\chi(k_0, t) \equiv P_{\nu\chi}(k_0, t)$ and for the distribution functions $N_{\nu}(k_0, t) \equiv \rho_{\nu\chi}(k_0, t)$ in the conduction/valence bands. For an undoped system in equilibrium, the initial conditions $P_\chi(k_0, 0) = 0$, $N_{\nu}(k_0, 0) = 0$, and $N_{\nu}(k_0, 0) = 1$ are assumed, neglecting thermal occupations. The integration of SBEs is performed on a 3D grid of $500 \times 500 \times 500$ points homogeneously distributed in the cube $(-\alpha_{\text{cut}} \omega/\nu, \alpha_{\text{cut}} \omega/\nu)_{XYZ}$. The minimum/maximum crystal momentum is defined by $\alpha_{\text{cut}}$, which in turn depends on the intensity of the pump wave. The time integration is performed with the standard fourth-order Runge-Kutta algorithm. From Eq. (17) follows the relation:

$$\frac{d \chi(t)}{dt} v^2 = \omega \left( \bar{t}, \xi_0, \frac{b \nu}{\omega}, \frac{\Gamma}{\omega} \right),$$

where $\bar{t} \equiv \omega t$, and $\omega \left( \bar{t}, \xi_0, \frac{b \nu}{\omega}, \frac{\Gamma}{\omega} \right)$ is a periodic (in case of an external monochromatic wave) dimensionless universal function that parametrically depends on the WSM–wave interaction parameters $\xi_0$, the scaled axial vector, and the scaled relaxation rate. Hence, by solving SBEs (16), performing the integral over $k_0$ (17) and taking Fourier transform ($\mathcal{F}\mathcal{T}$), the polarization-resolved high-harmonic spectrum is calculated as

$$I_\alpha = \left| \mathcal{F}\mathcal{T} \left( w_\alpha \left( \bar{t}, \xi_0, \frac{b \nu}{\omega}, \frac{\Gamma}{\omega} \right) \right) \right|^2, \quad \alpha = x, y, z.$$ (21)

For all calculations, the relaxation time is taken to be equal to half of the wave period $\Gamma^{-1} = T/2 = \pi/\omega$.

The typical photoexcitation of the Fermi-Dirac sea is presented in Fig. 1, where the density plot of the particle distribution function $N_\nu(k, t_f)$ after the interaction at the instant $t_f = 10 \Gamma$, as a function of dimensionless momentum components, for different orientations of the laser electric field strength are shown. As is seen from this figure, near the Weyl nodes we have an almost homogeneous excitation due to the singularity of the transition dipole moments. Far from the Weyl nodes the excitation pattern is defined by the anisotropy of the transition dipole moments (13) and (14).

In Fig. 2, the polarization-resolved HHG spectra in logarithmic scale for WSM in the strong-field regime for different orientations of the laser electric field strength are presented. From top to bottom we show the spectra for the $x$, $y$, and $z$ polarizations of the pump wave. As is seen from this figure, when the driving wave is polarized along $x$ direction, the odd harmonics are generated only along the laser polarization direction. However, when the wave is polarized along $y$ or $z$ directions, in addition to normal harmonics generated along the laser polarization, anomalous harmonics along perpendicular directions are also generated. As reflected from Fig. 2, anomalous harmonics are generated at the non-collinear arrangement of the electric field and Weyl node’s momentum separation vectors. This is the manifestation of the axionic field theory with the anomalous nonlinear electrodynamic effects. To understand how these findings are related to the non-trivial topology of WSM, let us derive another equivalent equation for the current (17) that explicitly includes Berry curvature (12). From Eq. (16), inserting expression for $\varepsilon_{\beta\alpha\chi}(k_0 + A) \rho_{\alpha\beta\chi}(k_0, t)$ into the equation for the current (17), taking into account the relation (15), electron-hole symmetry $V_{\nu\chi} = -V_{\chi\nu}$, and the integral of motion $N_{\nu\chi}(k_0, t) + N_{\chi\nu}(k_0, t) = 1$, we find

$$j_\alpha(t) = -2 \sum_{\chi k_0} V_{\chi\nu}^* N_{\nu\chi}(k_0, t)$$

$$-2 \text{Re} \sum_{\chi k_0} d^\nu_{\alpha\chi}(\chi, k_0 + A) \{ \partial_t P_{\chi}(k_0, t) + \Gamma P_{\chi}(k_0, t) \}$$

$$+ 2 \text{Re} \sum_{\chi k_0} i E(t) A^\chi(\chi, k_0 + A) d^\nu_{\alpha\chi}(\chi, k_0 + A) P_{\chi}(k_0, t)$$

$$+ \sum_{\chi k_0} \frac{1}{2} \epsilon_{abc} E^b(t) B^c(\chi, k_0 + A).$$

FIG. 1. Particle distribution function $N(k, t_f)$ (in arbitrary units) in the plane $k_z = 0$ after the interaction at the instant $t_f = \tau$ for WSM, as a function of scaled dimensionless momentum components $(k_x, \nu/\omega, k_y/\omega)$ for different orientations of the laser electric field strength. The wave-particle dimensionless interaction parameter is taken to be $\xi_0 = 0.5$, and the axial vector magnitude is chosen to be $b = \omega/\nu$. The Weyl nodes are located at $k_x/\omega = \pm 1$. 

FIG. 2. Polarization-resolved HHG spectra in logarithmic scale for WSM in the strong-field regime for different orientations of the laser electric field strength are presented. From top to bottom we show the spectra for the $x$, $y$, and $z$ polarizations of the pump wave.
The Weyl nodes are located at $k_\chi, v/\omega = \pm 0.5$. The axial vector to be infinity. As reflected from Fig. 1, near the Weyl nodes we have an almost homogeneous excitation for WSM in the strong-field regime for different axial vector magnitudes: $b v/\omega = 0.25$ and $b v/\omega = 0.5$. The wave-particle dimensionless interaction parameter is taken to be $\xi_0 = 1.0$.

At the first glance for each Weyl node taking into account unbounded linear dispersion of fermions one can make a naive shift of variable $k_{z\chi} = k_x - \chi b$, and make this integral to vanish. However, we should take into account singularity near $\pm b$ points as in the case of linear axionic field theory [28]. Therefore we need to choose a finite cut-off along the axial vector ($x$-direction), which can be sent to infinity at the end of calculations and can keep the cut-offs in the directions perpendicular to the axial vector to be infinity. As reflected from Fig. 1, near the Weyl nodes we have an almost homogeneous excitation due to the singularity of the transition dipole moments [13] and [14]. Hence, we can approximate the integral as

$$j_y \simeq \frac{2}{(2\pi)^3} E^z(t) N_{z;1}(k_{0w}, t)$$

where the summation over the repeated upper indices is implied. The first term in Eq. (22) is the ordinary intraband part of the current, the second and third terms define the interband part of the current, the fourth and fifth terms represent the topological part of the current. These terms are defined by the Berry curvature [12]. The fourth term is nothing but the anomalous Hall current [26, 27] and depends linearly on the field strength $E$, since $\sum k \chi = \sum k_\chi$. The last term in Eq. (22) is the nonlinear part of the anomalous Hall current that gives rise to anomalous harmonics perpendicular to the laser field strength directions: $e^{abc} E^b B^c = E \times B$. If the driving wave is polarized along the axial-vector $b$ ($x$-direction), then it is easy to see that the anomalous current along $y$ and $z$ directions turn out to be zero as monopole fields [12] of Weyl nodes cancel each other. On the other hand, when the driving wave is polarized along the $y$ or $z$ directions, then the $x$-component of the Berry curvature comes into play. Let us analyze for the concreteness the case of the $z$-polarized driving wave. In this case the anomalous Hall current can be written

$$j_y = \frac{E^z(t)}{(2\pi)^3} \int d^3k_0$$

$$\times \left[ \frac{(k_{0x} + b) N_{c;1}(k_{0}, t)}{\sqrt{(k_{0x} + b)^2 + k_{0y}^2 + (k_{0z} + A_z)^2}} - (b \rightarrow -b) \right].$$

The anomalous HHG spectra in logarithmic scale for WSM in the strong-field regime for different axial vector magnitudes: $b v/\omega = 0.25$ and $b v/\omega = 0.5$. The wave-particle dimensionless interaction parameter is taken to be $\xi_0 = 1.0$.

FIG. 2. The polarization resolved HHG spectra in logarithmic scale for WSM in the strong-field regime for different orientations of the laser electric field strength. The wave-particle dimensionless interaction parameter is taken to be $\xi_0 = 0.5$, and the axial vector magnitude is chosen to be $b = \omega/2v$. The Weyl nodes are located at $k_{\chi}, v/\omega = \pm 0.5$.
Hall current of WSM at high energies will be modified by a non-linear contribution from the axial-vector. In Fig. 3, the anomalous HHG spectra in the logarithmic scale for WSM in the strong-field regime, for different axial vector magnitudes are presented. The results for $b\nu/\omega = 0.25$ are multiplied by the factor 4. As is seen from Fig. 3, the intensities of anomalous harmonics are quadratically dependent on the momentum space separation of the Weyl nodes. This is consistent with our approximate result. This differs from the case of the lattice model [58] where the intensity of anomalous harmonics decreases with the increasing distance between the Weyl nodes. It is straightforward to see that for the normal harmonics with the shift of variable $k_{x\chi} = k_x - \chi b$ one can obtain the results independent on $b$. This is equivalent to the fact that the right and the left Weyl fermions are merged, we have a 4-component trivial massless Dirac fermion and, as a consequence, the anomalous harmonics vanish. In addition, the intensities of normal harmonics do not depend on the Weyl node’s momentum separation vector and resemble the results for a massless 3D Dirac fermion.

We now turn to an examination of the effect of the driving wave intensity on the HHG in WSM. We present the results of simulations for normal harmonics at different polarizations in Fig. 4. The intensities of normal harmonics $I_n$ do not depend on the Weyl node’s location. For the considered intensities the perturbation theory is not applicable, and in Fig. 4 we have a strong deviation from the power law for the intensities of harmonics. In particular, the intensities of the 5th, 7th, and 9th harmonics scale as $I_5 \sim \xi_0^3$, $I_7 \sim \xi_0^4$, and $I_9 \sim \xi_0^1$, respectively. Whereas they should show the $I_n \sim \xi_0^{5n}$ dependence in the perturbative limit. Besides, this figure shows that the intensities of the normal harmonics are almost independent of the pump wave polarization, which is connected with the isotropic linear dispersion of the Weyl fermions.

In Fig. 5, the HHG spectra for the anomalous harmonics for WSM in the strong-field regime for different orientations of the pump laser electric field strength at various wave-particle dimensionless interaction parameter $\xi_0$.

\[ \times \int_0^\infty k_{\perp} dk_{\perp} \int_{-\Lambda}^\Lambda dk_{0x} \int_0^{2\pi} d\phi \frac{k_{0x} + b}{[k_{\perp}^2 + (k_{0x} + b)^2]^{3/2}} \]

\[ = \frac{2}{(2\pi)^2} E^2(t) N_{e:1}(k_{0w}, t) \int_{-\Lambda}^\Lambda \text{sgn}(k_{0x} + b) dk_{0x} \]

\[ = \frac{b}{\pi^2} E^2(t) N_{e:1}(k_{0w}, t), \quad (24) \]

where $N_{e:1}(k_{0w}, t)$ is calculated near the Weyl node: $k_{0w} = (b, 0, 0)$. This is an interesting result that implies that the nonlinear anomalous Hall current is proportional to axial-vector as in the linear axionic field theory. But, this result is only valid for the unbounded linear dispersion of the Weyl fermions. If we consider a lattice model of WSM, the linear dispersion is valid only near the Weyl nodes, and integration is performed over the finite Brillouin zone. Therefore, the nonlinear anomalous

\[ \text{FIG. 4. The HHG spectra for the normal harmonics in logarithmic scale for WSM in the strong-field regime for different orientations of the pump laser electric field strength at various wave-particle dimensionless interaction parameter $\xi_0$.} \]
FIG. 5. The HHG spectra for the anomalous harmonics in logarithmic scale for WSM in the strong-field regime for different orientations of the pump laser electric field strength at various wave-particle dimensionless interaction parameter $\xi_0$. The Weyl nodes are located at $k_0\nu/\omega = \pm 0.5$.

numerically solved the semiconductor Bloch equations governing a WSM driven by a strong laser field in the length gauge and considered the HHG process depending on the Weyl node’s momentum separation vector and the driving wave intensity. Our results show that at the non-collinear arrangement of the electric and Weyl node’s momentum separation vectors, the anomalous harmonics are generated which are polarized perpendicular to the direction of the pump wave electric field. The intensities of anomalous harmonics are quadratically dependent on the momentum space separation of the Weyl nodes. When the right and the left Weyl fermions are merged, the anomalous harmonics vanish. In contrast to the anomalous harmonics, the intensities of normal harmonics do not depend on the Weyl node’s momentum separation vector. The dependences of the intensities of the normal and anomalous harmonics on the intensity of the driving wave are completely different, and for the moderately strong driving waves one can enter an extreme nonlinear regime of HHG. The results of the current investigation are not only of theoretical and academic importance but also will have significant implications for the rapidly developing area of modern extreme nonlinear optics of topological nanomaterials.

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