The role of time reversal symmetry and tilting in circular photogalvanic responses

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We study the role of time reversal symmetry (TRS) in the circular photogalvanic (CPG) responses considering chiral Weyl semimetal (WSM) while a finite CPG response is guaranteed by already broken inversion symmetry (IS) and mirror symmetries. The TRS broken WSM yields one left and one right chiral Weyl nodes (WNs) while there are two left and right chiral WNs for TRS invariant WSM. We show that these features can potentially cause the quantization of CPG response at higher values compared to the topological charge of the underlying WSM. This is further supported by the fact that Berry curvature and velocity behave differently whether the system preserves or breaks the TRS. We find that the quantization in CPG response is twice and four times the topological charge of the activated WNs for TRS invariant WSM while the quantization is directly given by the topological charge for the activated WNs in TRS broken case. This clearly suggests that the antisymmetric behavior of CPG response between two opposite WNs is lost for TRS invariant system referring to the unique transport signature of the above systems. Moreover, we find that the tilt can significantly modify the CPG response as velocity in the tilt direction changes which enters into the CPG tensor through the Fermi distribution function. Given these exciting outcomes, the second order CPG response emerges as a useful indicator to characterize the system under consideration. Following the low-energy theory, we analytically understand the numerical results as obtained from the lattice models. Furthermore, we investigate the momentum resolved structure of CPG response to relate with the final results and strengthen our analysis from the perspective of the lattice models.

I. INTRODUCTION

The Weyl Semimetals (WSMs)1–3 have drawn a huge attention in recent years due to their exotic properties that are mainly caused by the unusual Fermi arc surface states and chiral anomaly.4 It has been found in WSMs that non trivial band crossing occurs at an even number of discrete points in the Brillouin zone. These special gap closing points, protected by some crystalline symmetry, are referred as Weyl nodes (WNs) and they carry a topological charge (referred as Chern number) which is a quantized Berry flux through Fermi surface enclosing it in momentum space.4 It is important to mention here that upon breaking of either time reversal symmetry (TRS) or inversion symmetry (IS) or both of these symmetries in Dirac semimetals, each twofold degenerate Dirac cone reduces to two isolated WNs of opposite chiralities.5 In particular, there exist minimum two WNs of opposite chirality when the system breaks the TRS; four WNs are noticed in general for system with broken IS only.5 The conical spectrum and the point-like Fermi surface at the WN are the signature of an unfurled WSM namely, type-I WSMs. An interesting situation arises when large tilting of the Weyl cone results in a Lifshitz transition. This leads to a new class of materials called type-II WSMs, where the Fermi surface is no longer point-like. These WSM phases have been realized experimentally in several inversion asymmetric compounds (TaAs, MoTe2, WTe2).5,12

As expected, topological systems become fertile grounds for investigating various quantum topological electromagnetic responses.13–17 The chiral-anomaly related negative magnetoresistance, and the quantum anomalous Hall effect are the immediate upshot of the topological nature of WSM5,18–20. Apart from the electric transport, the exotic signatures associated with WSMs show up in the thermal responses which have been studied theoretically21–24 and experimentally,25–28. On the other hand, thanks to distinct behavior of density of states at the Fermi level, it has been shown that the electronic and thermal transport properties of type-II WSMs become markedly different from that of the associated with type-I WSMs.27–31 In addition to the linear optical responses, the higher order optical responses, such as circular photogalvanic effect (CPGE),32–35 second-harmonic generation34–39, are found to be very interesting for chiral topological crystals where the mirror symmetry is broken in addition to inversion symmetry resulting in non-degenerate WNs. Topological chiral semimetals (SMs) can be realized in many multifold fermions such as, the transition metal mono-silicides MSi (M = Co, Mn, Fe, Rh)34–39, double WSMs HgCr2Se4 and SrSi243–46 and triple-WSM like A(MoX)3 (with A = Rb, Tl; X = Te)47

It is important to have non-degenerate WNs to obtain interesting chiral transport behavior32,34,48. Very interestingly, the quantized behavior of CPG response, which is DC photocurrent switching with the sense of circular polarization of the incident light, happens to be a direct experimental probe to measure the Chern numbers in topological semimetals49. Very recently, a giant non-quantized photogalvanic effect and second-harmonic generation have been reported in non-centrosymmetric type II Weyl semimetal TaAs family,50–52 where degenerate WNs exist in the presence of mirror symmetry. The dipole moment of Berry curvature also leads to nonlinear Hall effect where non-quantized responses are observed.53

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Given the background on the higher order responses, we here probe the effect of TRS on the second order chiral transport namely, CPG response considering IS broken type-I and type-II WSM. The CPG response is found to exhibit quantized response proportional to the topological charge of the WNs when the underlying untitled WSM breaks TRS, IS, and mirror symmetries. The Pauli blocking mechanism controls the behavior of CPG response where only one WN would participate in the transport and the other WN with opposite chirality remains inactive. Our aim is to investigate the CPG response when the underlying WSM, preserving the TRS, possesses four WNs. The questions that we would like to precisely answer are the following: is CPG response always proportional to topological charge of the underlying WSM? does the number of WNs matter? and how can CPGE distinguishes between type-I and type-II WSMs with and without TRS? Much having explored on the non-quantized behavior of CPGE in presence of degenerate WNs, we believe that our analysis for the nature of quantized response in CPGE in presence of TRS happens to be the first study to the best of our knowledge.

In this work, we consider TRS broken and invariant type-I and type-II WSM to investigate the CPG response. We find that in general tilt can modify the CPG response as compared to the untitled case. For TRS broken WSM with two WNs shows quantized CPG response irrespective of the tilt except a few dissimilarities. The magnitude of quantization here is proportional to the topological charge of a single WN. Interestingly, for TRS invariant type-II WSM with four WNs, CPG response can only become quantized while for type-I it becomes non-quantized. The magnitude of quantization depends on both the number of WNs and topological charge associated with each WNs. Unlike the TRS broken case where CPG trace becomes quantized to two opposite values of same magnitude once the chemical potential is chosen close to the energies of two opposite chiral WNs, CPG trace exhibits quantization to two different values (twice and four times of topological charge) with opposite signs for TRS invariant WSM. In order to understand these results, we make resort to low-energy models where we show the Berry curvature and velocity for the activated WNs (by Pauli blocking mechanism) behave in a distinct manner. We also study the momentum resolved CPG trace to further appreciate the numerical results obtained from the lattice models.

The paper is organized as follows. In Sec. II we describe the CPG response and introduce the TRS invariant, TRS broken lattice model. We also analyze here the CPG trace as derived from the underlying low-energy model. Next in Sec. III we discuss our numerical results, obtained from the lattice model and understand them from the perspective of the low-energy model. Finally, in Sec. IV we conclude with possible future direction.

### II. Formalism and Model

#### A. Circular photogalvanic effect (CPGE)

The CPG injection current is a second order optical response when the system is irradiated with the circularly polarized light. It is defined as

\[ \frac{dJ_i}{dt} = \beta_{ij}(\omega) \left| E(\omega) \times E^*(\omega) \right|_j, \]

where \( E(\omega) = E^*(-\omega) \) is the circularly polarized electric field of frequency \( \omega \), \( i \) and \( j \) index are the direction of current \( J_i \) and circular polarized light field respectively. This optical activity is originated from the interband electronic transition. The tensor \( \beta_{ij} \) is purely imaginary and only non-zero if IS is broken. In a chiral topological semimetals where inversion and all mirror symmetries are broken, WNs appear at different energies. In this case the trace of \( \beta_{ij} \) is quantized for a finite range of frequencies. On the other hand, if the system possesses at least one mirror symmetry, all the diagonal components of \( \beta_{ij} \) vanish leaving the non-quantized CPG response from off-diagonal component of \( \beta_{ij} \). The CPG tensor \( \beta \) can be written in general as

\[ \beta_{ij}(\omega) = \frac{\pi e^3}{h V} \epsilon_{jkl} \sum_{k,n,m} \Delta f_{k,nm} \Delta v_{k,nm}^i \Delta v_{k,mn}^l r_{k,nm} r_{k,mn} \times \delta(h \omega - E_{k,mn}), \]

where \( V \) is the sample volume, \( E_{k,nm} = E_{k,n} - E_{k,m} \) and \( \Delta f_{k,nm} = f_{k,n} - f_{k,m} \) are the difference between \( n \)-th and \( m \)-th band energies and Fermi-Dirac distributions respectively, \( r_{k,nm} = i \langle n | \partial_k | m \rangle \) is the off-diagonal Berry connection and \( \Delta v_{k,nm}^i = \partial_k E_{k,nm}/\hbar = v_{i,n} - v_{i,m} \).

It is pertinent to discuss about the relation between the response coefficient and the incident applied intensity. Let’s consider the electric fields in the \( x-y \) plane, \( E = |E|(1, i, 0)/\sqrt{2} \). Therefore, the injection current induced in the \( z \) direction is given by

\[ \partial_t J_z = \beta_{zz} \left| E(\omega) \times E^*(\omega) \right|_z = i\beta_{zz} |E|^2 n_z \]

with \( n_z = (0, 0, 1) \). The total injection current can be obtained by adding up the contributions from the three orthogonal directions: \( \partial_t J_T = (\beta_{xx} + \beta_{yy} + \beta_{zz}) |E|^2 \). Under the reversal of polarization of the incident light i.e., \( i \rightarrow -i \), the injection current changes its sign. Therefore, by experimentally measuring the injection current, one can directly estimate the CPG response that is encoded in the CPG tensor \( \text{Tr}[\beta(\omega)] \).

The above CPG tensor reduces to a very tractable form for two band model where \( n, m = 1, 2 \). Following an analytical computation of CPG coefficient, one can find the of the trace CPG tensor \( \beta_{ij} \) for a two band model is...
given by
\[
\text{Tr}[\beta(\omega)] = \frac{i\pi e^3}{\hbar^2 v^2} \sum_k \Delta f_{k,12} \partial h_k \delta(h \omega - E_{k,12})
\]
\[
= \frac{i\pi e^3}{\hbar^2 v^2} \sum_k \Delta v_{k,12} \partial h_k \delta(h \omega - E_{k,12})
\]  
(4)

Here, \( \Delta v_{k,12} = v_{i,1} - v_{i,2} \) is the velocity difference between valence and conduction band; \( \Delta f_{k,12} = f_{k,1} - f_{k,2} \) is Fermi distribution function between valence and conduction band. \( \Omega_{i,k} = \epsilon_k \sum_{m \neq n} \tau^k_{n,m} \) is the \( i \)-th component of Berry curvature. It is to be noted here that \( \Delta f_{k,12} \), reducing to \( \pm 1 \), plays very crucial role in order to allow the participation of the WNs for a given value of chemical potential \( \mu \). This factor together with \( \delta \)-function determine the frequency dependence of the CPG response. We consider \( \omega > 0 \) to investigate meaningful transport properties.

Based on the linearized, un-tilted, isotropic model \( \mathbf{k} \cdot \mathbf{\sigma} \) for WNs, it has been shown that the CPG trace measures the Berry flux penetrating through a surface\(^{32}\). Therefore, the topological charge \( C \) of the WN, enclosed by the closed surface, results in a quantized CPG response. The quantization is observed in a certain frequency window which can be generically dependent on chemical potential \( \mu \). Another interesting feature encoded in the \( \delta \)-function is that CPG response shows quantized response as long as \( \omega \) is kept between two WN energies \( E_L \) and \( E_R \) i.e., \( 2|E_L| < \omega < 2|E_R| \) with \( E_{L,R} = E_{L,R} - \mu \). For \( \omega > 2|E_R| \), the other Weyl node contributes with opposite sign in the Berry flux and the quantization is observed in a certain frequency window.

To complete the discussion, we here present the Berry curvature associated with the topological WSM Hamiltonian. The Berry curvature of the \( m^{th} \) band for a Bloch Hamiltonian \( H(k) \), defined as the Berry phase per unit area in the \( k \) space, is given by\(^{32}\)
\[
\Omega^m_k = (-1)^m \frac{1}{4|N_k|} \epsilon_{abc} N_k \cdot \left( \frac{\partial N_k}{\partial k_b} \times \frac{\partial N_k}{\partial k_c} \right).
\]  
(5)

### B. Lattice Hamiltonian for IS and TRS broken WSM

We consider the following two band Hamiltonian for the single WSM\(^{32}\): \( H^I(k) = N_k \cdot \mathbf{\sigma} + N_{0,k} \sigma_0 \) with
\[
N_k = (t_1 \sin k_x, t_1 \sin k_y, -M + t_1 \sum_{i=x,y,z} \cos k_i),
\]
\[
= (N_{1,k}, N_{2,k}, N_{3,k}) \quad N_{0,k} = \gamma \sin k_z + t_2 \cos k_z,
\]  
(6)

where \( \sigma^0 \) is the 2 \( \times \) 2 identity matrix and \( \mathbf{\sigma} = (\sigma^x, \sigma^y, \sigma^z) \) the Pauli matrices. The Hamiltonian\(^{32}\) breaks TRS and IS: \( \mathcal{T} H^I(-k) \mathcal{T}^{-1} \neq H^I(k) \) with TR operator \( \mathcal{T} = \mathcal{K} \) where \( \mathcal{K} \) is complex conjugation; \( \mathcal{P} H^I(-k) \mathcal{P}^{-1} \neq H^I(k) \) with inversion operator \( \mathcal{P} = \sigma_x \). The energy eigenvalues of \( H^I(k) \) are \( E_{k,\pm} = N_{0,k} \pm |N_k| \) with \( |N_k| = \sqrt{N_{1,k}^2 + N_{2,k}^2 + N_{3,k}^2} \). For \( 1 < |M/t_1| < 3 \), the model exhibits a pair of WNs of chirality \( s \) at \( k_{s,z} = (0, 0, \pm k_0) \) with energies \( E_{k,s,z} = s \gamma \sin (k_0) + t_2 \cos k_0 \), where \( k_0 = \cos^{-1}(M/t_1 - 2) \). The right- \( (s = -1) \) and the left- \( (s = +1) \) handed WNs now appear respectively at \( E_{R} = \gamma \sin k_0 + t_2 \cos k_0 \) and \( E_{L} = -\gamma \sin k_0 + t_2 \cos k_0 \), producing a constant chiral chemical potential \( \mu_{ch} = (E_{R} - E_{L})/2 = \gamma \sin k_0 \), which is essential to obtain a non-zero CPG response. For \( t_2/t_1 \to 0 \) \( (t_2/t_1 \to 1) \), model becomes type-I (type-II) WSM. For \( M = 2 \) and \( t_1 = 1 \), the WNs appear at \( k_{s,z} = (0, 0, \pm \pi/2) \) associated with energies \( E_{R,L} = \pm \gamma \) (see Fig. 1).

The low energy Hamiltonian close to a WN with chirality \( s \) is given by
\[
H^I_{k,s} \approx s(\gamma - t_2 k_z) \sigma_0 + s k_x \sigma_x + s k_y \sigma_y + s k_z \sigma_z
\]  
(7)

The Berry curvature takes the form \( \Omega_{i} = \pm k_i/k^3 \) \( (i = x, y, z) \) with \( k = \sqrt{k_x^2 + k_y^2 + k_z^2} \). Here, \( \pm \) refers to the valence and conduction band. The velocity takes the form \( v_i = \pm s k_i/k \) \( (i = x, y) \) and \( v_z = \pm s(-t_2 + k_z/k) \). At the outset, we note that the term \( \sum_{x,y,z} \Delta v_{i} \Omega_{i} \) in CPG trace\(^{32}\) requires separate attention for opposite chiral WNs: \( \Delta v_{i} \Omega_{i} = k_i^2/k^4 \) for left chiral WN \( (s = +1) \) and \( \Delta v_{i} \Omega_{i} = -k_i^2/k^4 \) for right chiral WN \( (s = -1) \). For \( k = E_{R,L} \), we can consider the above low-energy model\(^{32}\). Using the expressions\(^{32}\) with \( \Delta f = 1 \), we then get
the CPG response as follows

$$\text{Tr}[\beta(\omega)] \approx \frac{e^3}{h^2} \int \frac{d\Omega}{(2\pi)^2} \int k^2 dk \sum_{i} \delta(\omega/2 - E_{12})$$

$$\approx \frac{e^3}{h^2} \int \frac{d\Omega}{(2\pi)^2} \int k^2 dk \sum_{i} \frac{\delta(\omega/2 - k)}{k^4}$$

$$= \frac{i e^3}{h^2} \int dS \cdot \Omega = is\frac{e^3}{h^2}C = is\beta_0$$

(8)

Here $d\Omega$ and $dS$ are the element of solid angle and surface area in a 3D geometry associated with spherical polar co-ordinate. The above formalism clearly shows that CPG trace measures the Berry flux penetrating through $S$ as discussed in Sec. [II A]. Therefore, the topological charge $C$ of the WN, enclosed by the closed surface, results in a quantized CPG response. Hence, from the linearized model (Eq. [7]), as derived from TRS broken Hamiltonian (6), one can find that CPG response changes with the chirality of the WNs. This clearly suggests that $\text{Tr}[\beta(\omega)]/i\beta_0$ acquires two opposite values when $\mu = E_R$ and $\mu = E_L$. The quantization window in terms of $\omega$ has already been discussed in Sec. [II A]. We would like to comment that linearized model gives us a hint about the quantization, the lattice model however needs to be considered to get the detail of the CPG response.

We shall now address the issue of tilt in the above expression (5). We note that the effect of tilt can only enter in the CPG response through the Fermi distribution function $f_T$. Interestingly, $\Delta_0$ and $\Omega_1$ both are tilt independent as tilt parameter $t_2$ appears in the $\sigma_0$ part of Eq. [7]. The momentum integration for tilted case would thus strongly depend on the apparently innocent factor $\Delta f$ that become $\pm 1$ for $T = 0$.

For completeness, we here discuss the explicit expressions of the Berry curvature $\Omega(k) = (\Omega_x(k), \Omega_y(k), \Omega_z(k))$ and the velocity $v(k) = (v_x(k), v_y(k), v_z(k))$ associated with Hamiltonian (6) are given by

$$\Omega_x = \pm \frac{\cos k_y \sin k_x \sin k_z}{|N_k|^3}$$

$$\Omega_y = \pm \frac{\cos k_x \sin k_y \sin k_z}{|N_k|^3}$$

$$\Omega_z = \pm \frac{- \cos k_y + \cos k_x (1 + \cos k_y (2 - \cos k_z))}{|N_k|^3}$$

$$v_x = \pm \frac{2 (2 - \cos k_x - \cos k_y) \sin k_x}{|N_k|}$$

$$v_y = \pm \frac{2 (2 - \cos k_x - \cos k_y) \sin k_y}{|N_k|}$$

$$v_z = \gamma \cos k_x - t_2 \sin k_z$$

$$\pm \frac{2 \cos k_y + \cos k_x - \cos k_z) \sin k_z}{|N_k|}.$$  

(9)

For a TRS broken WSM, we here find $\Omega(k) \neq -\Omega(-k)$. Here, $\pm$ refers to the valence and conduction band.

C. Lattice Hamiltonian for IS broken and TRS invariant WSM

![Figure 2](image)

FIG. 2. The energy dispersion $E_k$ for IS broken WSMs are shown as function of $k_x$ and $k_z$ for type-I (a) and type-II (b). We repeat (a) and (b) considering $k_y = 0$ in (c) and (d). Two Weyl points at $k_z = \pm \pi/4$ are separated in energy $E_R - E_L = t_2(\delta - 1)$. The parameters are considered here are following: $\delta = 2.0$, $t_1 = 1.0$, $t_2 = 0.002$ for type-I and $t_2 = 0.3$ for type-II.

The two band model for single WSM considered here is given by $\mathcal{H}^{II}(k) = N_k \cdot \sigma + N_{0,k} \sigma_0$ with

$$N_k = t_1 [\cos k_0 - \cos k_y + \delta (1 - \cos k_z)],$$

$$t_1 \sin k_z, t_1 [\cos k_0 - \cos k_z] + \delta (1 - \cos k_z)],$$

$$(N_{1,k}, N_{2,k}, N_{3,k})$$

$$N_{0,k} = t_2 (2 \cos (k_z + k_y) + \delta \cos (k_x - k_y)),$$

(10)

where, $t_1$ and $t_2$ are the hopping parameters, $\delta \neq 1$ is a constant. The Hamiltonian (10) breaks IS but preserves TRS; $T \mathcal{H}^{II}(-k)T^{-1} = \mathcal{H}^{II}(k)$ and $\mathcal{P} \mathcal{H}^{II}(-k)\mathcal{P}^{-1} \neq \mathcal{H}^{II}(k)$. The energy eigenvalues of $\mathcal{H}_{k,\pm}^{II}$ are $E_k, \pm = N_{0,k} \pm |N_k|$ with $|N_k| = \sqrt{N_{1,k}^2 + N_{2,k}^2 + N_{3,k}^2}$. For $t_2 = 0$ and $\delta > 1$, four gapless points arise in the $k_z = 0$ plane and without any loss of generality we can consider $0 < k_0 < \pi$. The right-handed $(s = +1)$ WNs are located at $k_{1,2,3} = \pm (k_0, k_0, 0)$ and the left-handed $(s = -1)$ WNs are located at $k_{1,2,3} = \pm (k_0, -k_0, 0)$. When $t_2 \neq 0$, $N_{0,k}$ causes shift in energies of the WNs of opposite chiralities. The right and the left-handed WNs now appear respectively at $E_R = t_2 [\cos (2k_0) + \delta]$ and $E_L = t_2 [1 + \delta \cos (2k_0)]$, producing a constant chiral chemical potential $\mu_{ch} = (E_R - E_L)/2 = t_2(\delta - 1)\sin^2 k_0$, which is essential to obtain a non-zero CPG response. One can get type-I and type-II WSM by tuning the ratio of $t_2/t_1$. For $t_2/t_1 < 0.01$, two bands meet at four type-I WNs. For $t_2/t_1 > 0.01$, the WNs start to tilt in the $x$-direction and we
have four type-II WNs. Considering $k_0 = \pi/4$, one finds two left chiral WNs at $k_{1,2}^\perp = \pm (\pi/4, -\pi/4, 0)$ and two right chiral WNs at $k_{1,2}^\parallel = \pm (\pi/4, \pi/4, 0)$ with energies $E_L(E_R) = t_2(z_2)$. The low energy Hamiltonian close to a given chiral node with chirality $s$ is given by $\mathcal{H}_{k,s} \approx n_s\sigma x_0 + t_1(\mathbf{k}\cdot \mathbf{\sigma}) + t_2(1-k_y k_y)$ with $n_{x,z} = -1, 0$. For completeness, the explicit expressions of the Berry curvature, velocity difference and the curvature contribution in the momentum integration of CPG trace at $k_{1,2}^\perp$ become identical. To be precise, we find $\Omega = k^2/k^3$ and $\Delta v_\parallel = k^2/k^3$ for both the right chiral WNs. On the other hand, for both the left chiral WNs at $k_{1,2}^\perp$, we find $\Omega = -k^2/k^3$. Interestingly, $x$ and $y$ components of velocity difference change their sign at these two left chiral WNs, i.e., $\Delta v_\parallel = \pm k^2/k^3$ for $k = k_{1,2}^\perp$ with $i = x, y$ while $\Delta v_\parallel = \mp k^2/k^3$ remains unaltered. Therefore, one can infer from the low-energy minimal model that for TRS invariant (broken) WSM, the Berry curvature and velocity difference around the WNs associated with two different chiralities behave differently (similarly) as far as the individual components are concerned. These further result in distinct behavior of CPG response while $\mu$ is considered close to the WNs of opposite chirality.

Let us do the analysis for $\mu \approx E_R$. Here, we have to consider the low-energy model in the vicinity of two WNs at $k_{1,2}^\perp$. Therefore, we take into account both of their contribution in the momentum integration of CPG trace while evaluating the quantity $\sum_i x_{i,z} \Delta v_i \Omega_i$. It appears that $\Delta v_i \Omega_i = k^2/k^3$ for both WNs. Considering these right chiral low-energy Hamiltonians, one can find the CPG response \textbf{[4]} with $\Delta f = 1$, as follows:

$$\text{Tr}[\beta(\omega)] \approx \frac{e^3}{\hbar^2} i \int \frac{d\Omega}{(2\pi)^3} \int k^2 dk \sum_{i} x_{i,z} \Delta v_i \Omega_i \frac{\delta(\omega - E_{R,12})}{2}$$

$$= \frac{e^3}{\hbar^2} i \int \frac{d\Omega}{(2\pi)^3} \int k^2 dk \sum_{i} x_{i,z} \frac{k^2}{k^4} \frac{\delta(\omega - k/2)}{2}$$

$$= i \frac{e^3}{\hbar^2} \oint_S d\mathbf{S} \cdot \mathbf{\Omega} = \frac{e^3}{\hbar^2} C = i\beta_0$$

(11)

Following the similar line of argument based on low-energy model, the CPG response for $\mu \approx E_L$ (i.e., left chiral WNs) is found to be:

$$\text{Tr}[\beta(\omega)] \approx \frac{e^3}{\hbar^2} i \int \frac{d\Omega}{(2\pi)^3} \int k^2 dk \sum_{i} x_{i,z} \Delta v_i \Omega_i \frac{\delta(\omega - E_{L,12})}{2}$$

$$= \frac{e^3}{\hbar^2} i \int \frac{d\Omega}{(2\pi)^3} \int k^2 dk \Delta v_i \Omega_i \frac{\delta(\omega - k/2)}{2}$$

$$= \frac{e^3}{\hbar^2} i \int \frac{d\Omega}{(2\pi)^3} \int k^2 dk \frac{k^2}{k^4} \frac{\delta(\omega - k/2)}{2}$$

$$= \frac{e^3}{\hbar^2} i \oint_S d\mathbf{S} \cdot \mathbf{\Omega} = \frac{e^3}{\hbar^2} C = i\eta_0$$

(12)

In the above calculation, one has to include the two WNs at $k_{1,2}^\parallel$ to evaluate the quantity $\sum_{i} x_{i,z} \Delta v_i \Omega_i$ using the associated with the left chiral low-energy model. A close inspection would suggest that $\Delta v_\parallel \Omega_i = \pm k^2/k^4 (i = x, y)$ and $\Delta v_\parallel \Omega_y = -k^2/k^4$. As a result, $\sum_{i} x_{i,z} \Delta v_i \Omega_i$ reduces to $-k^2/k^4$. We consider $k = k \cos \theta$ and the angular integration $\int d\Omega$ is weighted by $\cos^2 \theta$ leading to the factor $\eta C < C$ as $\eta < 1$. This is in contrast to the result obtained in Eq. (11) for right chiral WNs at $\mu \approx E_R$, where regular angular integral $\int d\Omega$ leads to $C$. By comparing Eq. (11) and (12), one can find that the low-energy theory refers to a situation where left and right chiral WNs result in a non-antisymmetric behavior for TRS invariant system. By contrast, TRS broken low energy model exhibits anti-symmetric behavior between left and right chiral WNs (see Eq. (8)). Therefore, the number of WNs for a given chirality and the specific detail of the Berry curvature, velocity difference both become crucial in determining the CPG response.

For completeness, the explicit expressions of the Berry curvature $\Omega(k) = (\Omega_x(k), \Omega_y(k), \Omega_z(k))$ and the velocity $\mathbf{v}(k) = (v_x(k), v_y(k), v_z(k))$ associated with the Hamiltonian \textbf{[10]} is given by

$$\Omega_x = \pm \left[ \left( \frac{-\delta + (\cos k_0 + \delta - \cos k_x) \cos k_y}{|N_k|^3} \right) \sin k_y \right]$$

$$\Omega_y = \pm \left[ \left( \frac{-\delta + (\cos k_0 + \delta - \cos k_y) \cos k_x}{|N_k|^3} \right) \sin k_x \right]$$

$$\Omega_z = \pm \left[ \left( \frac{-\delta + (\cos k_0 - \cos k_y) \cos k_x}{|N_k|^3} \right) \sin k_x \right]$$

$$v_x = \pm \left[ \left( \frac{\cos k_0 - \cos k_x + \delta (1 - \cos k_z)}{|N_k|} \right) \sin k_z \right]$$

$$v_y = \pm \left[ \left( \frac{\cos k_0 - \cos k_y + \delta (1 - \cos k_z)}{|N_k|} \right) \sin k_z \right]$$

$$v_z = \pm \left[ \left( \frac{\delta (2 \cos k_0 - 2 \cos k_x - \cos k_x - \cos k_y)}{|N_k|} \right) \sin k_z \right]$$

(13)

For a TRS invariant WSM, we here find $\Omega(k) = -\Omega(-k)$. Here, $\pm$ refers to the valence and conduction band.

III. RESULT AND DISCUSSIONS

Having discussed the formalism to compute the CPG tensor, we now investigate it for IS broken WSMs. To begin with, we numerically estimate CPG trace for the TRS broken type I Weyl semimetal \textbf{[8]} as shown in Fig. 3 (a)-(b). We here consider the chemical potential for both inside and outside region of two non-degenerate WNs. The WNs with topological charge $C_{R,L} = \mp 1$ appear at $E_{R,L} = \pm 0.8$ for $k_0 = \pm \pi/2$. Both the WNs with energies $E_L$ and $E_R$ are equally spaced below and above for the
chemical potential $\mu = 0$ i.e., $E_R' = E_L'$ with $|E_{R,L} - \mu| = E'_{R,L}$. We find that CPG trace vanishes irrespective of the value of frequency for $\mu = 0$. On the other hand, for $\mu = \pm 0.8$, our investigation shows that the quantization in CPG trace at $\pm 1$ starts from $\omega = 0$ and lasts until $\omega \approx 2.0$. However, the CPG trace decreases for $\omega > 2.0$ and vanishes around $\omega \approx 3.2$. One can thus infer that CPG response is dependent on $|E'_{R,L} - E'_{R,L}|$. Precisely, the region of the quantization is found inside the following frequency window $2|E'_{L}| < \omega < 2|E'_{R}|$.

We shall now discuss the CPG response when $\mu$ is away from the WN energies. For the chemical potential $\mu = -0.3$, inside between two WNs with $|E'_{L}| < |E'_{R}|$, the frequency window for the quantitation at $\pm 1$ is $1.0 < \omega < 1.5$ (see Fig. 3(b)). For $\mu = 0.3$, the value of the quantization reverses within the same energy windows as $E'_{R,L} > |E'_{R,L}|$. The underlying reason is that the transport is maximally governed by the nature of the activated WN i.e., the magnitude (sign) of quantization depends on the topological charge (chirality) of that WN. However, we find that the CPG trace becomes finite within the frequency window $2|E'_{L}| < \omega < 2|E'_{R}|$. The frequency above (below) which CPG trace starts (ends) showing quantized behavior decreases toward zero when $E'_R$ and $E'_L$ are maximally deviated from each other. As a result, for $\mu = \pm 0.8$ ($\pm 0.3$), one can find largest (smallest) frequency window for quantization. When the chemical potential is outside the energy window between the two WNs, but close to any of the WNs within the linear band touching region, the CPGE is also found to be quantized (see Fig. 3(b)). Expectedly, the quantized value depends on the topological charge of the activated WN. But when $\mu \gg E_R, E_L$, i.e., far away from the non trivial band crossing, the CPG trace becomes non-quantized acquiring smaller value $< 1$. Importantly, we find anti-symmetric behavior of CPG response symmetrically placed around $\mu = (E_L + E_R)/2$.

In contrary, for the IS broken case as shown in Fig. 3(c), CPG trace is never found to be quantized in any of the above circumstances. One can observe sharp peak for certain values of chemical potential otherwise, it remains zero throughout the whole frequency range. We note that $E_L, E_R \to 0$ leading to the fact that the frequency window becomes non-existent in practice. Interestingly, the anti-symmetric nature of CPG tensor with $\mu$ being positive and negative is also lost. It can acquire values such as $> +1$ ($< -1$) which is larger (smaller) than the topological charge of a single WN. We note that the total number of Weyl points present in the system is four. Therefore, non-quantized CPG trace can be in principle larger (smaller) than $+1$ ($-1$). Based on our analysis in these two species of type-I models, CPG trace is able to capture the symmetry mediated transport in a distinct way. For TRS broken model, the quantized value is proportional to the charge of the Weyl point while for TRS invariant model, the quantization is absolutely absent, however, the magnitude can be larger than the topological charge. One can infer that in order to obtain quantized response of CPG trace for type-I WSMs, the breaking of TRS plays a very crucial role. However, the most essential condition to obtain quantized response is to have a substantial energy gap between WNs of different chiralities. For TRS invariant model (10), the above criterion is violated $|E_R - E_L| = t_2(\delta - 1) = 0.002$ eV while TRS broken model (6), it is satisfied $|E_R - E_L| = 2\gamma = 1.6$ eV. In order to understand this phenomena in more detail, we below investigate the type-II analogue of these models.

Figure 3(a)-(b) show the CPG trace for IS and TRS broken tilted type-II WSM. Here the quantization is only obtained when the chemical potential is kept near to the energy of one of the WNs. For $\mu = \pm 0.8$ and $\pm 0.75$, the CPG trace is quantized with values $\mp 1$ within the frequency windows $0.2 < \omega < 1.2$. This quantization

![Figure 3](image-url)
window for type-II WSM is almost half as compared to that of the for type-I WSM with the same value of chemical potential. The tilt modifies the available states near the Fermi surface (otherwise point like for type-I untilted case) appearing in the CPG trace through the Fermi distribution function \( (\Delta f_{12}) \) associated with the \( k \) modes in BZ. The tilt thus imprints its effect by eventually normalizing the frequency window within which CPG response acquires quantized value. Interestingly, when \( E_R' = E_L' \), CPG does not to vanish like type I. For the IS broken case, the quantized value is noticed to be 2 times and 4 times the topological charge of the activated WNs when \( \mu \) is set around \( E_L, E_R \) respectively.

Now, we analyze the CPG response for IS broken type-II WSM where we find the quantized response for \( E_L < \mu < E_R \) kept close to the WN energy \( E_L = t_2 = 0.7 \) and \( E_R = t_2\delta = 1.4 \) (see Fig. 4 (c)). This behavior remain unaltered when \( \mu \) is close to \( E_L \) or \( E_R \) but outside the energy window set by these energies (Fig. 4 (d)). Comparing with type-II TRS broken WSM, we find that TRS invariant type-II WSM behaves in an identical way as far as the quantization is concerned. Surprisingly, CPG becomes quantized to two different values \(-2 \) and \(+4\) for \( \mu \) close to \( E_L \) and \( E_R \), respectively. This suggests that the anti-symmetric nature of the CPG response is lost considering \( \mu \) being symmetrically placed around \( (E_L + E_R)/2 \). This is in complete contrast to the TRS broken case where the magnitude of quantized value depends only on the charge of the activated Weyl point. One can find that there exist two left (right) chiral Weyl points at \( E_L (E_R) \) with topological charge \( C_L = -1 \) (\( C_R = +1 \)). When \( \mu \) is set close to \( E_L \), the transport is governed by both of these two left chiral WNs and they contribute additively resulting in CPGE to be proportional to \( 2C_L \). On the other hand, when \( \mu \) is close to \( E_R \) where there exist two right chiral WNs with \( C_R = +1 \), CPGE is found to be quantized to \( 4C_R \) instead of \( 2C_R \). This can be understood in the following way that activated WNs contribute differently i.e., the product of the Berry curvature and velocity difference in the CPG trace at left and right chiral WNs are not identical for TRS invariant model. Whereas, for TRS broken model, the product of the Berry curvature and velocity difference in behave in an identical fashion for two opposite chiral WNs which leads to perfectly anti-symmetric nature of CPG trace. We can thus comment that the transport in type-II TRS broken WSM is intrinsically differnet from the TRS invariant model type-II WSM.

![FIG. 4. Behavior of CPG trace for TRS broken type-II WSM in (a) and (b); IS broken type-II WSM in (c) and (d) for both inside (\( E_L < \mu < E_R \)) and outside (\( \mu < E_L, \mu > E_R \)) region. For TRS broken case, the quantization in CPGE to two opposite values, that are given by the topological charge of the activated WN, is clearly observed in when \( \mu \) is set only around any of the Weyl point energy (\( E_{R,L} \)). Interestingly, when \( \mu \) is close to \( E_L \), CPG does not to vanish like type I. For the IS broken case, the quantized value is noticed to be 2 times and 4 times the topological charge of the activated WNs when \( \mu \) is set around \( E_L, E_R \) respectively.](image-url)
magnitude is also noticed for the WN at \( k_z = (0, 0, \pi/2) \) with \( \mu = 0.8 \).

We would now analyze the TRS invariant case where four Weyl points are found: two left chiral WNs at \( k_z^{1,2} = \pm (\pi/4, -\pi/4, 0) \) with \( E_L = t_2 \) and two right chiral WNs at \( k_z^{1,2} = \pm (\pi/4, \pi/4, 0) \) with \( E_R = t_2 \delta \). When \( \mu \approx E_L \), the left chiral nodes contribute maximally to the CPG tensor \( \text{Tr}[\beta] \approx \sum_k \sum_{i=1}^{12} A(k_i, x, \mu \approx E_L) \delta(\omega - E_{k_{i,12}}) \). A careful analysis with \( A(k_{i,12}, x, \mu \approx E_L) \), considering the low energy model, suggests that \( \text{Tr}[\beta] \approx -\sum_k \Delta v_x \Omega_x \delta(\omega - E_{k_{i,12}}) \). On the other hand, \( \mu \approx E_R \), the right chiral nodes contribute maximally to the CPG tensor \( \text{Tr}[\beta] \approx \sum_k \sum_{i=1}^{12} A(k_i, y, \mu \approx E_R) \delta(\omega - E_{k_{i,12}}) \). Following the similar line of argument, one can find \( \text{Tr}[\beta] \approx \sum_k (\Delta v_x \Omega_x \pm \Delta v_y \Omega_y \pm \Delta v_z \Omega_z) \delta(\omega - E_{k_{i,12}}) \). Therefore, the low energy model can successfully predict the distinct behaviour in CPGF tensor when \( \mu \) is close to left and right chiral WNs. Interestingly, in the TRS broken case all three component of CPG tensor i.e., \( \beta_{xx}, \beta_{yy} \) and \( \beta_{zz} \), contribute irrespective of the fact that whether \( \mu \approx E_L \) or \( E_R \). For TRS invariant WSM, this analogy breaks which results in exhibiting different quantization magnitude for \( \mu \approx E_L \) and \( \mu \approx E_R \). This is in sharp contrast to the TRS broken case where the magnitude of quantization for CPG response becomes identical for both the chemical potential \( \mu \approx E_L \) and \( \mu \approx E_R \).

In order to anchor this analysis, we show \( A(k_x, k_y, k_z = 0, \mu) \) numerically from the lattice model \( (10) \) in Fig. 5 (c) and (d) for \( \mu = E_L = 0.7 \) and \( \mu = E_R = 1.4 \), respectively. We find that the sign of \( A \) reverses between \( k_z > \pi/4 \) and \( k_z < -\pi/4 \) with \( \mu = 0.7 \). While for \( -\pi/4 < k_z < \pi/4 \), \( A(k_x, k_y, k_z = 0, \mu = E_L) \approx 0 \). \( A \) exhibits kink close to the Weyl point \( k_z^{1,2} = \pm (\pi/4, -\pi/4, 0) \) for \( \mu = 0.7 \) rendering the fact that these two left chiral nodes actively participate in CPGF quantization which is found to be \( 2C_L = -2 \). While for \( \mu = 1.4, A > 0 (\sim 0) \) for \( k_z > -\pi/4 (< -\pi/4) \); however, the value of \( A \) increases for \( k_z > \pi/4 \) as compared to the value of \( A \) for \( -\pi/4 < k_z < \pi/4 \). Here, \( A \) exhibits kinks close to the right chiral Weyl point \( k_z^{1,2} = \pm (\pi/4, \pi/4, 0) \) suggesting the fact that these WNs actively participate in the quantization in CPGF response which has the value \( 4C_R = 4 \).

The momentum integration of \( A \) over the BZ for TRS broken WSM becomes negative (positive) when \( \mu = 0.8 \) (\( \mu = -0.8 \)) as shown in Fig. 5 (a) (Fig. 5 (b)). This is directly reflected in the behavior of CPG tensor for \( \mu = \pm 0.8 \). Once \( \mu \) reduces (increases) from 0.8 (–0.8), the magnitude of \( A \) decreases in the BZ for \( k_y > 0 \). For \( \mu = 0 \), \( A \) becomes vanishingly small in the BZ. As a result, the quantization is observed for \(-0.8 \leq \mu \leq 0.8 \) except \( \mu = 0 \). These above nature of the momentum distribution of \( A \) is also qualitatively valid for the tilted type-II case. However, unlike the type-I case, the tilt can destroy the quantization when \( \mu \) is away from \( \pm 0.8 \) within the window \(-0.8 \leq \mu \leq 0.8 \). The non-zero value of CPG tensor for \( \mu = 0 \) in type-II case is due to the anisotropic nature of the dispersion which is imprinted in \( A \) through the Fermi distribution function \( \Delta f_{12} \).

The lattice analysis of \( A \) further reveals that it can have both positive and negative contributions in the BZ for TRS invariant WSM with \( \mu = 0.7 \) as shown in Fig. 5 (c). Upon increasing \( \mu > 0.7 \), one can find that \( A \) reduces for \( k_z < -\pi/4 \). \( A \) increases and becomes positive when \( \mu \) reaches 1.4 when \( k_z < -\pi/4 \). In intermediate zone \( -\pi/4 < k_z < \pi/4 \), \( A \) increases when \( \mu \) increases from 0.4 to 1.4. For \( \mu = 1.4 \), \( A \) only acquires positive values for \( k_z > \pi/4 \) as shown in Fig. 5 (d). From the momentum distribution of \( A \) for the TRS invariant WSM, it is evident that \( A \) does not show any anti-symmetric behavior as observed for TRS broken WSM when \( \mu \) is kept at two different Weyl point energies \( E_L \) and \( E_R \). This again points towards the fact that CPGF response can be very different for TRS broken and TRS invariant WSM in terms of the quantization. On the other hand, for type-I TRS invariant WSM, \( A \) turns out to be vanishingly small but anti-symmetric with respect to \( k_x = 0 \)-plane in the BZ. As a result the CPG response becomes characteristically different from the tilted case.

Exact quantization in CPG trace is predicted from the \( k \cdot \sigma \) model. The quantization can be destroyed due to several lattice effect. Away from the WNs, band bending causes the deviation of CPGF response from quantized value. This quantization is clearly observed when \( \mu \) is set close the WN energy. On a general note, we can infer that for type-II WSM, the band bending near the WNs affects the quantization more compared to type-I.
The band bending is more prominent in type-II and that can result in the non-linear correction to the quantization. In addition, we would like to note for experimental observability that the prefactor $\beta_0$ of Eq. (1) is large in comparison to ordinary CPG trace magnitudes. Considering typical relaxation times, one can find that the other metallic or insulating contributions are less than an order of magnitude as compared to the quantized WN contribution. As a result, we believe total CPG trace observed in experiment can signal the quantization.

IV. CONCLUSION

We consider TRS invariant and TRS broken WSM to study the CPG response where the energies $E_L$ and $E_R$, associated with the left and right chiral Weyl points, are different from each other $E_L \neq E_R$. The motivation is to analyze the effect of TRS on the quantization while the IS and mirror symmetries are already broken for both these WSMs. We consider general tilted lattice Hamiltonian which allows us to additionally investigate the effect of tilted dispersion in the CPG response. There exist only two WNs of opposite chirality in TRS broken system, while at least four WNs of opposite chiralities are present in TRS invariant WSM. Therefore, when the number of WNs for a given chirality is more than unity that could become an interesting situation to study. To be precise, a relevant question here is that how does the quantization depend on the number of WNs. In this work, we show that quantization for TRS invariant single WSM can be 2 and 4 times the topological charge of the activated WNs (see Fig. 4). This feature is not observed for TRS broken WSM as there exists only one WN for a given chirality (see Fig. 5). In addition, CPG response is able to distinguish a type-II from a type-I WSM in general.

In particular, the Berry curvature and the velocity difference play very important role in determining the behavior of CPG trace. The tilt is not able to change the Berry curvature for anisotropic case from the isotropic case, however, velocity along the tilt direction can become very different from the isotropic case. The effect of tilt enters through the Fermi distribution function in the CPG trace as the velocity difference remains independent of the tilt parameter. As a result, CPG response for type-II is distinguishably different from type-I. For example, in the TRS broken type-I case, CPG trace behaves exactly opposite to each other when $\mu$ is symmetrically chosen around $\mu = (E_L + E_R)/2$. This feature is not observed for the tilted type-II case. Moreover, CPG response can acquire values larger than the magnitude of the topological charge in presence of the tilting. Interestingly, in our present case, type-II TRS invariant can only exhibit quantization in CPG trace unlike to the type-I counterpart where $E_L \approx E_R$. The magnitude of quantization for $\mu$ close to $E_L$ and $E_R$ strongly depends on Berry curvature and velocity around the left and right chiral WNs. In the TRS broken WSM, the value of quantization for $\mu \sim E_L$ is just opposite to that of the for $\mu \sim E_R$. For TRS invariant these two values of quantization are different from each other as the Berry curvature and velocity (as well as the velocity difference) behave differently for left and right chiral WNs. We find the above features numerically analyzing the lattice models and then, supplement them using the low-energy model derived around the WNs.

We believe that our observation can be tested experimentally due to availability of the setup. It would be interesting to study the TRS broken and invariant chiral multi-WSM having non-linear anisotropic dispersion. The band bending causes the CPGE to deviate from quantized behavior. The role of TRS and band bending are two important aspects that can be studied in future in chiral SMs.

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