Irradiated three-dimensional Luttinger semimetal: A factory for engineering Weyl semimetals

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We study the interaction between elliptically polarized light and a three-dimensional Luttinger semimetal with quadratic band touching using Floquet theory. In the absence of light, the touching bands can have the same or the opposite signs of curvature; in each case, we show that simply tuning the light parameters allows us to create a zoo of Weyl semimetallic phases. In particular, we find that double and single Weyl points can coexist at different energies, and they can be tuned to be type I or type II. We also find an unusual phase transition, in which a pair of Weyl nodes form at finite momentum and disappear off to infinity. Considering the broad tunability of light and abundance of materials described by the Luttinger Hamiltonian, such as certain pyrochlore iridates, half-Heuslers and zinc-blende semiconductors, we believe this work can lay the foundation for creating Weyl semimetals in the lab and dynamically tuning between them.

Introduction.- Topological phases of matter have attracted tremendous interest since the discovery of topological insulators. Topological protection of their edge and surface states is the hallmark of these systems, and leads to applications ranging from quantum computation to robust transport and exotic superconductivity [1, 2]. In contrast to topological insulators, which are gapped phases of matter like most topological phases, it has been shown recently that gapless phases of matter can be topological as well [3-9]. Among them, Weyl semimetals (WSMs) have been particularly attractive due to their unconventional properties such as the chiral anomaly [11, 12], negative magnetoresistance [10, 11] and anomalous Hall effect [5, 8]. Experimental observation of these phases in TaAs [11, 13, 14] and photonic crystals [15] has ignited further interest in exploring these systems.

Very recently, new types of WSMs, namely, type-II and multi-WSMs were also discovered [16-18, 20]. The defining feature of type-II Weyl points is that the dispersion around them is strongly anisotropic, such that the slope changes sign along some directions. As a result, the Weyl nodes become the touching points between electron and hole Fermi surfaces, and result in properties different from those of type-I WSMs. For example, there are indications that the chiral anomaly depends on the relative direction of the magnetic field and the tilt of the cone, but the issue is still under debate [16, 17]. Moreover, unlike in type-I WSMs, the anomalous Hall effect can survive in type-II WSMs under certain conditions even when the nodes are degenerate [21]. On the other hand, multi-WSMs occur when the monopole charges of Weyl points are higher than 1, and can be either type-I or type-II [18, 20]. In general, the search for Weyl semimetallic phases has been a vigorous field of research lately, and proposals have been put forth to engineer these phases in a tunable way by shining light on Dirac semimetals [25, 26], band insulators [20], stacked Graphene [31], line-nodal semimetals [29, 32] and crossing-line semimetals [24, 26]. Finally, proposals have been made to create tunable WSMs in pyrochlore iridates with Zeeman fields [43, 52].

FIG. 1: Phase diagram for 3D Floquet Luttinger semimetal. Critical line (Isotropic limit): diagonal red line with two lower (w1) and two higher (w2) Weyl points on the k_z axis; phase I: 4w1 + 2w2 , blue, where for bands bending oppositely (similarly), the 4w1 are type-I (type-II) denoted by phaseI = 1(2)&2. The notation 1(2) denotes type-I (type-II) Weyl nodes in the respective phase. The first number is the type of lower and the second number after & indicates the type of the higher nodes. Phase III: 4w1 + 2w2, orange, where for bands bending oppositely (similarly), the 2w2 are type-I (type-II) and denoted by phaseIII = 1-2&2. Phase II, green, shows the transient phases between phase I and III where the flat bands in the k_z-direction (k_z - k_y plane) for bands bending in opposite (same) directions, as well as merging and splitting of lower and upper nodes in k_y and k_z - k_x planes, respectively, occur. "TPD" denotes the triply degenerate point, which exists only for circular light.

In this work, we expand the horizons for creating tunable WSMs, by computing the band structure of a three-dimensional Luttinger semimetal with quadratic band
touching irradiated by elliptically polarized light using Floquet theory. We find Weyl nodes of different charges (±1 and ±2), Weyl nodes of different types (type-I and type-II), and several phases which contain more than one class of Weyl nodes. We also stumble upon a situation where a pair of Weyl nodes form at infinity, and rapidly come in and merge with other nodes at finite k. In a regularized lattice model, this pair would form at the edge of the Brillouin zone. Crucially, given the bare band structure, all these phases can be accessed by simply changing the properties of the light, making this system highly tunable. Fig. 1 summarizes the results of this paper. We expect these results to hold for real systems described by the Luttinger Hamiltonian [33], such as the zinc-blend semiconductors GaAs, HgTe, α-Sn etc. and a class of pyrochlore iridates [34, 37] studied recently.

Model and Formalism.- We begin with an isotropic version of the Luttinger Hamiltonian [33],

\[ H = \frac{1}{2} \int_k e^i(k) \left( (\lambda_1 + \frac{5}{2} \lambda_2)k^2 - 2\lambda_2(J,k)^2 - \mu \right) c(k), \]

where \( \lambda_{1,2} \) are positive constants, \( k = \{k_x, k_y, k_z\} \), \( e(k) = (c_{3/2k}, c_{1/2k}, c_{-1/2k}, c_{-3/2k})^T \), \( J = \{J^x, J^y, J^z\} \) are effective spin-3/2 operators, and \( c_{0k} \) denotes a fermion annihilation operator with momentum \( k \) and \( J_z \) quantum number \( m \). The energy dispersions are \( E(k) = (\lambda_1 \mp 3\lambda_2)k^2 - \mu \) for the \( j = 3/2 \) and the \( j = 1/2 \) bands, respectively. Time-reversal and inversion symmetries ensure that the four bands come in doubly degenerate pairs due to Kramer’s theorem. The degenerate bands curve the same (opposite) way for \( \lambda_2 < 2\lambda_1 \) (\( \lambda_2 > 2\lambda_1 \)), as depicted in Fig. 2. When both bands bend the same way, Eq. (1) is widely used to model heavy- and light-hole bands in zinc-blende semiconductors [37]. Many properties of such a dispersion have been studied in the literature, including a recent study on the realization of fully gapped topological superconductivity with p-wave pairing which has states with exotic cubic and linear dispersions coexisting on the surface [38, 39]. On the other hand when bands bend oppositely, the above model is relevant for certain pyrochlore iridates as well as for some doped half-Heusler alloys such as LaPtBi [40, 42]. Various aspects of this scenario have been explored as well, such as the phase diagram in the presence of electronic interactions [43], the effect of anisotropy [44] and superconductivity [45, 46]. Systems with higher effective spins and winding numbers have also attracted interest in the context of multi-weyl phases [47] and the investigation of the spin quantum Hall plateau transition on the surface of topological superconductors with general winding numbers [48].

FIG. 2: Energy dispersion of Eq. (1) for (a) \( \lambda_1 = 0.1 \) and \( \lambda_2 = 0.5 \) with \( J = 3/2 \) (red) bending down \( J = 1/2 \) (blue) bending up, and (b) \( \lambda_1 = 1.8 \) and \( \lambda_2 = 0.5 \) where both bands bend up. Note that the bands are doubly degenerate.

Here, we study another aspect of this model. By employing machinery from Floquet theory, we investigate light-matter interactions in this model in both band-bending scenarios. We consider periodic driving induced by laser light with a general vector potential \( \mathbf{A}(t) = (A_x \cos(\omega t), A_y \eta \sin(\omega t), 0) \), \( \eta = \pm 1 \) corresponds to right-handed and left-handed polarizations of the light, respectively, and \( A_\lambda \propto E_\lambda / \omega \), where \( E_\lambda \) is its electric field. The time-dependent Hamiltonian can be written as \( H(k, t) = \sum_n H_n(k) e^{in\omega t} \), where \( H_{\pm n}(k) = \frac{1}{\tau} \int_0^\tau H(k, t) e^{\pm in\omega t} dt \).

The effective time-independent Hamiltonian in the high frequency limit, as dictated by Floquet theory, is [23, 27],

\[ H_{\text{eff}}(k) = H_0 + \sum_{n \geq 1} \frac{[H_{+n}, H_{-n}]}{n\omega} + O\left(\frac{1}{\omega^7}\right). \]

where,

\[ H_1 = (\lambda_1 + \frac{5}{2} \lambda_2)k \cdot \mathbf{A} - 2\lambda_2 (\mathbf{J} \cdot \mathbf{J} \cdot \mathbf{A} \mathbf{J}) \]

\[ H_2 = \frac{1}{4} ((\lambda_1 + \frac{5}{2} \lambda_2) \mathbf{A}^2 - 2\lambda_2 (\mathbf{J} \cdot \mathbf{A})^2) \]

\[ H_{-n} = H_n^\dagger \]

and \( \mathbf{A} = (A_x, \eta A_y, 0) \). The Floquet perturbation series is controlled by parameter \( \gamma \equiv \lambda e^2 E^2 / \hbar \omega^3 \), where \( \lambda \) is either \( \lambda_1 \) or \( \lambda_2 \) which are of the same order of magnitude and have units of inverse mass, \( E \) is the magnitude of the electric field of the incident light and \( e \) is the speed of light in the medium. Clearly, \( \gamma \ll 1 \) at high enough frequencies, thus controlling the Floquet expansion. We discuss the estimation of this parameter in the real experiments in the concluding section. In the meantime, we work in the units \( e = \hbar = 1 \). We first analyze the limit of circular polarization, which is the only case can be fully studied analytically. Then, we analyze the general case of elliptical polarization.

Circularly polarized light.- Since \( H \) is quadratic in \( k \), \( H_n = 0 \) for \( n > 2 \) in Eq. (2). The terms coming from \( n = \pm 2 \) are momentum-independent, and it is their competition with the K-dependent terms arising from \( n = \pm 1 \) that proves to be essential in realizing the various WSMs.
In other words, the leading order correction in $A$ is insufficient, and it is necessary to go to a higher order. For circularly polarized light, rotational symmetry ensures that Weyl points appear only on the $k_z$ axis, which makes extracting the salient features of the model analytically possible. For $k_x = k_y = 0$, the effective Hamiltonian reads

$$H_{\text{eff}}(k_z) = H_0(k_z) + \frac{2i\eta A^2 \lambda_2^2}{\omega} \left(-k_z^2[\{J_x, J_z\}, \{J_y, J_z\}]\right)$$

$$+ \frac{A^2}{8} \left(J_y^2 - J_x^2, \{J_x, J_y\}\right),$$

with dispersions of $E_{1,\pm} = (\lambda_1 + 2\lambda_2) k_z^2 \pm (3A^2 \lambda_2^2 \eta (A^2 - 8k_z^2))/2\omega - \mu$ and $E_{2,\pm} = (\lambda_1 - 2\lambda_2) k_z^2 \pm (3A^2 \lambda_2^2 \eta (A^2 + 8k_z^2))/2\omega - \mu$. Note that introduction of circularly polarized light has broken time-reversal symmetry and lifted the double degeneracy of the bands. Inversion symmetry survives, though, because only even powers of the light amplitude enter $H_{\text{eff}}$. The four non-degenerate bands intersect in various pairs, giving rise to Weyl nodes at $K_1 = (0, 0, \pm A/2\sqrt{2})$ and $K_2 = (0, 0, \mp A^2\sqrt{3\lambda_2}/\omega/2)$. We can compute the monopole charge of each node by writing an effective low energy Hamiltonian around in the form $H_k \propto n(k) \cdot \sigma$ and using,

$$W_n = \int_S d^2k \epsilon^{ijk} n_i (\partial_j n \times \partial_k n)$$

where $n$ is a unit vector and the integration is over a surface $S$ surrounding the node. We obtain $W_n = \pm 1$ and $W_n = \pm 2$ for $K_1$ and $K_2$ respectively. This is a remarkable result, that single and double-Weyl nodes coexist at different energies, thus allowing us to access both dynamically by tuning the chemical potential. As is clear, the positions of single Weyl points are only a function of the light parameters while the locations of the double-Weyl points also depend on the band structure parameter, $\lambda_2$. Moreover, for circularly polarized light, there is a special point in parameter space, namely, $A_m = \pm \sqrt{\omega/6\lambda_2}$ where the two types of nodes merge and form a triply degenerate point (TDP).

Fig. 3(a-d) shows the evolution of the band structure with the light intensity, for a representative set of parameters with $\eta \lambda_2 > 0$ in a scenario with bands bending oppositely. This corresponds to evolution along the $A_x = A_y$ line in Fig. 1. Two pairs of nodes appear (Fig. 3a) as soon as light is turned on. The nodes higher (lower) in energy are type-II (type-I), have monopole charge $\pm 1$ ($\pm 2$) and occur at $K_1$ ($K_2$). On increasing $A$, the lower nodes flatten along $k_z$ (not shown) and transition into type-II nodes, before merging with the upper nodes at the TDP at $A = A_m$ (Fig. 3b). On further increasing $A$, the bands cross, and the charge $\pm 2$ nodes end up being higher in energy than the charge $\pm 1$ nodes (Fig. 3c). The latter then transitions back from type-II to type-I (Fig. 3d). In summary, the upper nodes are always type-II, while the lower nodes evolve from type-I to type-II and back to type-I. Naturally, the bands hosting the lower Weyl nodes flatten twice during this evolution, once at each transition between type-I and type-II characters. The charges are $\pm 1$ ($\pm 2$) for the upper (lower) nodes for low intensity, and the correspondence gets reversed as $A$ is tuned across the TDP.

Elliptically polarized light.—Now, we turn to the more general case of elliptically polarized light, i.e., $A_x \neq A_y$. 

FIG. 3: Evolution of the Weyl nodes with light amplitude $A$. (a)-(d) show $A = 2, 2.58, 2.7$ and 3, respectively for bands bending oppositely. For (e)-(h), we used $A = 2, 2.58, 2.7$ and 5, respectively, to show the type-II to type-I phase transition for high enough intensity with both bands bending in same direction. $\lambda_1 = 0.1, \lambda_2 = 0.5$ ($\lambda_1 = 1.8, \lambda_2 = 0.5$) are used for bands bending oppositely (similarly). $\omega = 20, \mu = 0$ and $\eta = 1$ is used for all of the plots.
The phase diagram is much richer when the incident light is anisotropic in the field’s amplitudes. In the following, we analyze various driven phases in the two band-bending possibilities shown in Fig. 2.

Let us first study Eq. (4) when the bands are bent oppositely. The phase evolution for this case is depicted in Fig. 4. In describing the evolution, we keep $A_y$ fixed at a high or a low value, and tune $A_x$ from 0 to $A_y$.

Let us first look at high $A_y$. For large anisotropy with $A_y \gg A_x$, there are 4 type-I nodes of unit monopole charge on the $k_y-k_z$ plane and 2 type-II nodes of charge $\pm 2$ at higher energies on the $k_x$-axis (Fig. 4a and 6a). On increasing $A_x$, the two higher nodes split into four type-II nodes of unit charge in the $k_x-k_z$ plane (Fig. 4b and 6b). On further increasing $A_x$ a pair of type-II nodes of unit charge come in on the $k_z$ axis from $k_z = \pm \infty$ while there are still 4 nodes in $k_y-k_z$ plane (Fig. 4e and 5a).

The new node at $k_z > 0$ presumably has a monopole charge opposite to that of the two nodes in the $k_y-k_z$ plane at $k_z > 0$; an analogous condition holds for $k_z < 0$ with all monopole charges reversed. Finally, the nodes in each triplet merge to yield two type-II nodes of charge $\pm 1$ (Fig. 5) on the $k_z$ axis. These nodes charge character from type-II to type-I, accompanied by the flattening of one of the bands participating in the nodes (Fig. 4d), and survive in this form up to the circularly-polarized limit (Fig. 4e). In the meantime, the four higher nodes remain type-II with unit charge, but merge into two type-II, charge $\pm 2$ nodes in the limit of $A_x = A_y$. Therefore we end up of 2 higher (type-II, $\pm 2$) and lower (type-I, $\pm 1$) nodes as explained in the previous section (Fig. 4e).

It should be noted that the TDPs are absent for elliptical polarization. However, for lower $A_y$, situation is different. In this case the situations of Fig. 4(b-d) do not happen. In another words, for lower $A_y$, the upper nodes do not split, while the merging of lower four points happens near the isotropic limit. Moreover, no flat-line occurs, and the upper nodes (type-II) have $\pm 2$ charges.

When both bare bands bend in same direction, the phase diagram undergoes almost the same evolution as the case with bands bent oppositely. In particular, it starts with four lower and two higher nodes, which, after a series of merging and splitting, yields a phase with two lower and four higher nodes. Finally, in the circular polarization limit, the higher nodes merge, leaving only two lower and two higher nodes. Therefore
are couple of differences. Firstly, as we mentioned in the previous section, nodes are type-II for most amplitude ranges. The second, instead of a flat line along \( k_x \), there is a "flat-band" in the \( k_x - k_z \) plane. The flat-line along \( k_z \) does happen, but only for very large \( A_y \). This is consistent with the type-II to type-I transition that was found to occur at high intensities in the isotropic limit for bare bands bending in the same direction.

**Discussion, experimental considerations and concluding remarks.** - In this work we have studied the Floquet theory of the three-dimensional Luttinger semimetal with quadratic band touching points. We have found that depending on the orientation of bands and light parameters, both type I and II Weyl nodes with single and double monopole charges at different energies can be generated. In particular we arrive at the following main results:

- When the incident light is circularly polarized, we have solved the problem analytically and have obtained two nodes with charge \( \pm 1 \) and two other nodes with \( \pm 2 \) at different energies. For both band bending scenarios, the higher nodes are always type-II while the lower ones can be type-I or II depending on light parameters. We found that at a certain light intensity, both pairs of nodes merge to form two TDPs. This is a special point which exists only for circularly polarized light and is a function of both light and band structure parameters.

- For the elliptically polarized light, we have only solved system numerically. For both bands bending scenarios, for large anisotropy, \( A_x \ll A_y \), there are two higher nodes on the \( k_z \) axis and four lower nodes in \( k_y - k_z \) plane. Then, when the \( A_y \) is held fixed at a small value and \( A_x \) is increased, the four lower nodes merge around \( A_z \sim A_y \). However, for high enough \( A_y \), on increasing \( A_x \), the lower Weyl nodes merge and then tilt back and turn into a flat-line (flat-band) for bare bands bending oppositely (similarly) and make two nodes. On the other hand the higher nodes deform to nearly flat lines and then split to four nodes in \( k_z - k_y \) plane which finally merge at isotropic limit.

Therefore, we conclude that the Luttinger semimetal with parabolic dispersion provides a master platform for realizing various types of WSMs from type I to type II with four nodes or two nodes, as well as single and double monopoles. Remarkably, we found that single and double-Weyl can coexist at different energies, so either ones can be accessed through controlled doping of the system and tuning of laser light. To the best of our knowledge this is the only system that reported so far with this level of tunability for broad range of possible Weyl phases. In addition, irradiated Luttinger semimetals is the only example so far discovered with Weyl node with different monopole charges coexist, making it feasible for the possible realizations of both single and double WSMs from a system with no Weyl nodes. There have been some recent studies \[25, 26\], where photo-induced multi-Weyl phases were generated from crossing-line systems.

The Luttinger Hamiltonian describes a wide range of materials from semiconductors to pyrochlore iridates and half-Heuslers which are accessible experimentally, unlike the other semimetals such as Dirac, loop-node, or linked semimetals, where experimental examples are rare or non-existent. Therefore, this work might facilitate the experimental realizations of photoinduced WSMs. Using \( \lambda_2 = 4.2/m_0 \) for HgTe, where \( m_0 \) is the bare electron mass, \( h\omega = 120\text{meV} \) and an electric field of \( E_0 = 2.5 \times 10^5\text{V/m} \) – typical values for pump-probe experiments \[50\] – we estimate the perturbation parameter \( \gamma = \lambda e^2 E^2/h\omega^3 \approx 10^{-10} \), so the Floquet expansion is
certainly well-controlled. The only word of caution is that, as with all three-dimensional Floquet systems, our proposal only works for films thin enough for the electric field to penetrate the system substantially.

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