**Photoinduced topological phase transition from a crossing-line nodal semimetal to a multiple-Weyl semimetal**

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We propose a simple scheme to construct a model whose Fermi surface is comprised of crossing-line nodes. The Hamiltonian consists of a normal hopping term and an additional term which is odd under the mirror reflection. The line nodes appear along the mirror-invariant planes, where each line node carries the quantized Berry magnetic flux. We explicitly construct a model with the $N$-fold rotational symmetry, where the $2N$ line nodes merge at the north and south poles. Photoirradiation induces a topological phase transition. When we apply photoirradiation along the $k_z$ axis, there emerge point nodes carrying the monopole charge $\pm N$ at these poles, while all the line nodes disappear. The resultant system describes anisotropic multiple-Weyl fermions.

**Introduction:** Weyl semimetal is one of the hottest topics in condensed matter physics.\(^{[1,2]}\) It is protected by a monopole charge in the momentum space.\(^{[3]}\) Multiple Weyl semimetal is a generalization of a Weyl semimetal which has a monopole charge larger than the unit charge.\(^{[4,5]}\) There exist another class of novel semimetals. They are line nodal semimetals whose Fermi surfaces form one-dimensional line.\(^{[6,7]}\) A line node is protected by a quantized Berry magnetic flux. Recently, line nodal semimetals are generalized into two species. One is a loop node forming a nontrivial link such as the Hopf link.\(^{[8,9]}\) The other is a crossing-line node, where several line nodes cross at a point.\(^{[10,11]}\)

Photoirradiation is a powerful tool to modify the band structure.\(^{[12]}\) According to the Floquet theory an additional term emerges due to the second-order process of photoirradiation. A typical example is the generation of a Weyl point from a Dirac semimetal.\(^{[13,14]}\) It is shown that a Weyl node can also be generated by applying photoirradiation to a loop nodal semimetal.\(^{[15,16]}\)

In this paper, we first propose a simple scheme to construct models for crossing-line nodal semimetals. We then investigate how a crossing-line nodal semimetal is modified by way of photoirradiation. The model Hamiltonian consists of a normal hopping term and a mirror-odd interaction term. A line node emerges on the mirror-invariant plane. Each line node is topologically protected by the quantized Berry magnetic flux. Explicitly, we construct an $N$-fold rotational symmetric model, where the crossing of $2N$-fold line nodes occurs at the north pole and also at the south pole. There are no magnetic monopoles at these poles. Next, we derive a photoinduced term based on the Floquet theory. It induces a topological phase transition. Indeed, by applying photoirradiation along the $z$ direction, the Fermi surface is found to disappear by the emergence of gap except for two nodal points carrying the $N$ ($-N$) units of the monopole charge at the north (south) pole. The resultant system is the anisotropic $N$-fold multiple-Weyl semimetal. On the other hand, by applying photoirradiation perpendicular to one of the loop node, the resultant Fermi surface turns out to be comprised of this loop node and point nodes. Otherwise, only the point nodes appear.

**Model:** A prototype of line nodal semimetals is given by the model

$$H(k) = f_x(k)\sigma_x + f_z(k)\sigma_z,$$  \hspace{1cm} (1)

whose energy spectrum reads

$$E(k) = \pm \sqrt{f_x^2(k) + f_z^2(k)}. \hspace{1cm} (2)$$

The Fermi surface is given by the two conditions $f_x(k) = 0$ and $f_z(k) = 0$, each of which produces a two-dimensional surface. The intersection of the two surfaces consists of lines and/or points in general. Namely we obtain line nodes and/or point nodes in general. For simplicity we consider the following case: (i) The condition $f_z(k) = 0$ generates an ellipsoid, which is rotational symmetric around the $k_z$ axis and centered at the origin ($k = 0$). (ii) The condition $f_x(k) = 0$ generates planes sharing the $k_z$ axis with each other. Furthermore we require that $f_x(k)$ is odd under the mirror operation $M_x$ with respect to each plane, where the index $\alpha$ denotes the direction normal to the plane. For example, if $f_x(k)$ is odd for the mirror reflection with respect to the $k_yk_z$ plane, $M_x f_x(k_x, k_y, k_z) M_x^{-1} = -f_x(-k_x, k_y, k_z)$, we have a zero-energy solution at $k_z = 0$ since $M_x f_x(0, k_y, k_z) M_x^{-1} = -f_x(0, k_y, k_z)$.

A key observation is that, when there are $N$ mirror-odd planes, there emerges the crossing of $2N$ line nodes. For example, by assuming the $N$-fold rotation symmetry, the lattice Hamiltonian is given by \(^{[1]}\) together with

$$f_x(k) = t \sum_{j=1}^{N} \cos (d_j^x \cdot k) + t_z \cos k_z - m', \hspace{1cm} (3)$$

$$f_z(k) = \lambda' g(k_z) \prod_{j=1}^{N} \sin (d_j^z \cdot k),$$

where $d_j^x = (\cos [j \pi/N], \sin [j \pi/N], 0)$ and $d_j^z = (\sin [(2j + 1) \pi/(2N)], \cos [(2j + 1) \pi/(2N)], 0)$. We have included a function $g(k_z)$ to allow the freedom of introducing additional crossing-line nodes perpendicular to the $k_x$ axis such as in \(^{[12]}\) for the cubic symmetric model. The summation runs over the nearest neighbor sites. The Fermi surface is given by the cross section of the $N$ planes and the ellipsoid. They are $2N$ line nodes which cross at the north and south poles. We show Fermi surfaces for $N = 2$ and $N = 3$ in Figs.\(^{[1]}\) (a1) and (b1), respectively. (Actually, we present almost zero-energy surfaces $E = \delta$ with $0 < \delta \ll t$. We note that the lattice structure is possible in the real space only for $N = 2$ and 3. The lattice with $N = 2$ forms a layered square.
The corresponding continuum theory is given by

\[ H = \left[ a \left( k_x^2 + k_y^2 \right) + c k_z^2 - m \right] \sigma_x + \lambda g \left( k_z \right) \text{Re} (k_z^N) \sigma_z \]  

(4)

with \( a = -N t / 4, \) \( c = -t_z / 2, \) \( m = m' + N t + t_z \) and \( \lambda = \lambda' / 2^{N-1}. \) For example, for the case of \( N = 2, \) there are two mirror planes \( M_{x+y} \) and \( M_{x-y}. \) A simplest representation is \( f_z = k_x^2 - k_y^2, \) whose zero-energy solution is given by the two planes \( k_x = k_y \) and \( k_y = -k_x. \) For the case of \( N = 3, \) there are three mirror planes determined by \( f_z = k_x^3 - 3k_x k_z^2. \) We show the Fermi surfaces in Figs.1(a2) and (b2). The Fermi surfaces obtained in the continuum theory are found to be almost the same as those obtained in the lattice model. Hence, we use the continuum theory in the following.

With the use of the eigenfunction \( |\psi\rangle \) of the Hamiltonian \( H, \) we may calculate the Berry connection as

\[ A_i \left( k \right) = \left. -i \langle \psi | \partial_i |\psi\rangle \right| = \frac{f_x \partial_i f_x - f_y \partial_i f_y}{2 \left( f_x^2 + f_y^2 \right)} = \frac{1}{2} \partial_i \Theta \]  

(5)

with \( \partial_i = \partial / \partial k_i, \) where \( f_x = f \cos \Theta, f_y = f \sin \Theta \) and...
\( f = \sqrt{f_x^2 + f_z^2} \): We show the stream plot of the Berry connection for \( N = 2 \) and 3, where vortex and antivortex structures are observed around the line nodes in the constant \( k_z \) plane, as in Figs.1(b1) and (d1). A pair of vortex and antivortex annihilates at the north and south poles as in Figs.1(b2) and (d2). Each line node is topologically protected since the Berry phase along the line nodes is quantized to be \( \pm \pi \),

\[
\oint A_j dk_j = \int \nabla \times A \, ds = \pm \pi.
\]  

(6)

The Berry curvature \( B = \nabla \times A \) is strictly localized along the line node. Indeed, we can explicitly check this by the direct calculation,

\[
B_i (k) = \varepsilon_{ijk} \partial_j A_k = \pm \pi \sum \delta (f_x) \delta (f_y).
\]  

(7)

Namely, the Berry magnetic flux is present along each line node, while the Berry curvature is strictly zero away from the line nodes. Consequently a line node is topologically protected.

**Photoirradiation parallel to the \( k_z \) axis**: We proceed to investigate a topological phase transition due to the \( \sigma_z \) term induced by photoirradiation. The following formulas hold for any function \( g(k_z) \) in \( \mathbb{R} \). We summarize the Floquet theory on photoirradiation. First, we irradiate a beam of circularly polarized light along the \( z \) direction. We take the electromagnetic potential as \( A_{\text{EM}}(t) = (A \cos \omega t, A \sin \omega t, 0) \), where \( \omega \) is the frequency of light with \( \omega > 0 \) for the right circulation and \( \omega < 0 \) for the left circulation. The effective Hamiltonian due to the second order process of photoirradiation is given by\textsuperscript{15}:

\[
\Delta H_{\text{eff}} (k, A_{\text{EM}}) = \frac{1}{\hbar \omega} [H_{-1} (k, A_{\text{EM}}), H_{+1} (k, A_{\text{EM}})].
\]  

(8)

It is explicitly evaluated to be

\[
\Delta H_{\text{eff}} (k, A_{\text{EM}}) = f_y \sigma_y,
\]  

(9)

where

\[
f_y = -2n \alpha \omega g (k_z) \text{Im}(k_+^N) \]  

(10)

with \( \alpha = (eA)^2 / (\hbar \omega) \). The second-order perturbed process produces the term \( f_y (k) \sigma_y \) due to the commutation relation \( [\sigma_z, \sigma_x] = i \sigma_y \). By including this term into the Hamiltonian we find

\[
H (k) = f_x (k) \sigma_x + f_y (k) \sigma_y + f_z (k) \sigma_z,
\]  

(11)

while the energy is modified as

\[
E (k) = \pm \sqrt{f_x^2 (k) + f_y^2 (k) + f_z^2 (k)}.
\]  

(12)

Now the condition \( f_y (k) = 0 \) should be imposed as the zero-energy condition additionally to \( f_x (k) = f_z (k) = 0 \). In general, there is no intersection between three surfaces, and the system becomes an insulator. However, there are several cases where crossing-line nodes are reduced to points nodes, as shown in Figs.1(a3) and (c3). The Fermi surface consists of only two point nodes at the north and south poles, \( (k_x, k_y, k_z) = (0, 0, k_z) \) with \( k_z = \pm \sqrt{m/c} \). In the vicinity of these points, we have

\[
f_z \approx \pm 2 \sqrt{mc} (k_z \mp \sqrt{m/c}).
\]  

(13)

The Hamiltonian with photoirradiation is given by

\[
H = \pm 2 \sqrt{mc} (k_z \mp \sqrt{m/c}) \sigma_z + \lambda g (k_z) \text{Re}(k_+^N) \sigma_z - 2na \alpha \omega g (k_z) \text{Im}(k_+^N) \sigma_y.
\]  

(14)

In particular, when \( 2na (eA)^2 = \hbar \omega \) and \( g (k_z) = 1 \), the Hamiltonian is reduced to that of the multiple-Weyl fermion,

\[
H = \lambda (k_+^n \sigma_+ + k_-^n \sigma_-) \pm 2 \sqrt{mc} (k_z \mp \sqrt{m/c}) \sigma_z,
\]  

(15)

and otherwise it is that of the anisotropic multiple-Weyl fermion. The Berry curvature is calculated as

\[
B_i (k) = \varepsilon_{ijk} \sin \Theta (\partial_j \Theta \partial_k \Phi - \partial_k \Theta \partial_j \Phi)
= \varepsilon_{ijk} (\partial_j f \times \partial_k f) \cdot f
\]  

(16)

where \( f = (f_x, f_y, f_z) \) with \( f_x = f \cos \Theta \sin \Theta, f_y = f \sin \Theta \sin \Theta, f_z = f \cos \Theta \). It describes monopoles with the charges \( \pm N \) at the north and south poles. We illustrate the Berry curvature around the north pole for \( N = 2 \) and 3 in Figs.1(b3) and (d3) for the case of \( g (k_z) = 1 \), where the presence of the monopoles is observed as a source or a sink of the Berry magnetic flux. We conclude that, by applying photoirradiation along the \( z \) direction, the Fermi surface changes from the nodal crossing lines to the two nodal points carrying the \( N \) (\( -N \)) units of the monopole charge at the north (south) pole.

**Photoirradiation perpendicular to the \( k_z \) axis**: We next apply photoirradiation perpendicular to the \( k_z \) axis. We explicitly study the tetragonal symmetric model \( (N = 2) \) and the trigonal symmetric model \( (N = 3) \). Here we set \( g (k_z) = 1 \) in \( \mathbb{R} \).

The lattice Hamiltonian of the tetragonal symmetric model with \( N = 2 \) is given by

\[
f_x = t (\cos k_x + \cos k_y) + t_z \cos k_z - n',
\]  

\[
f_z = -\lambda (\cos k_x - \cos k_y).
\]  

(17)

We inject photoirradiation along the \( \phi \) direction with \( A_{\text{EM}}(t) = (-A \sin \phi \cos \omega t, A \cos \phi \cos \omega t, A \sin \omega t) \). The effective Hamiltonian induced by photoirradiation along the \( \phi \) direction is given in the continuum theory by

\[
f_y = -\alpha \lambda t z k_z (k_x \sin \phi + k_y \cos \phi).
\]  

(18)

Solving \( f_x = f_z = f_y = 0 \), we obtain the Fermi surface.

When \( \phi = \pi / 4 \) or \( -\pi / 4 \), there emerge a loop node along the \( k_x = k_y \) plane or the \( k_x = -k_y \) plane, and two zero-energy points emerge at the two points \( (k_x, k_y, k_z) = \)
modes emerge. Namely, a loop node emerge only when the direction of photoirradiation is perpendicular to the loop node. Figs.1(c5) and (d5).

\begin{equation}
\begin{aligned}
f_x &= t (\cos k_x + \cos k_y + \cos k_z) - m', \\
f_z &= \lambda' \sin k_x \sin k_y \sin k_z,
\end{aligned}
\end{equation}

where we have set \( g(k_z) = \sin k_z \) in [3]. We illustrate the Fermi surface of the lattice model and the continuum model in Fig.2(a) and (b). Photoirradiation applied along the \( z \) direction induces the term

\begin{equation}
f_y = \alpha \lambda t k_x (k_x^2 - k_y^2)
\end{equation}

in the continuum theory. Solving \( f_x = f_y = 0 \), we obtain a loop mode given by \( k_x^2 + k_y^2 = 2(3t - m)/t \) and \( k_z = 0 \). Additionally anisotropic double-Weyl points emerge at the north and south poles, carrying the monopole charge \( \pm 2 \). We illustrate the Fermi surface in Fig.2(c).

Discussion: Crossing-line nodal semimetals with the cubic symmetry are realizable in CaTe and Cu3PdN according to recent first principles calculations in Ref.13 and Ref.14, respectively. It is also shown that LaN has a crossing line node, which is topologically identical to the cubic symmetric model in Ref.10. Furthermore, a hexagonal hydride, \( \text{YH}_3 \), has a crossing-line nodes with \( N = 3 \), as shown in Ref.15. It is an interesting problem to search further materialization of crossing-line node semimetals.

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