Unambiguous detection of topological nodes via Berry monopole indicators

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The unambiguous detection of the band topology for topological nodal systems remains an urgent problem in this field. Usually in experiments this relies on the detection for the topological edge modes, which may requires the high demands for the preparation and purifications of the materials and may give ambiguities. In this work, we propose a new approach towards the unambiguous detection of the bulk band crossing nodes of topological nodal systems without evolving the edge mode. The spirit of our proposal is to couple our targeted Hamiltonian to an weak external field $A$ with a spatial varying texture in a compact manifold which may lead to the variation of the wavevector $k$, and the system will have a response current $J$. When the field $A$ is close to the nodal point, the current $J$ has the same texture as $A$, indicating that we may turn the measurement for the bulk topological band crossing nodes into the measurement for the spatial texture of $J$, and a Berry monopole indicator indicator $w$ can be constructed to indicate the distance between the field $A$ and the band crossing node. Our findings provide an new perspective for the detection of band topology and pave the way for the further theoretical and experimental studies.

Introduction.— Topological semimetals (TSMs) have been attracting tremendous research interests due to its fundamental physics and promising device applications [1–3]. Generally TSMs can be classified into Dirac semimetals with four-fold degenerate Dirac nodes [4, 5], Weyl semimetals with two-fold degenerate Weyl nodes [6], and nodal line semimetals with continuous line of nodes inside the first Brillouin zone (BZ) [7–10]. A simplest two-band Weyl point model can be written as $\hat{H} = (k - b) \cdot \sigma$, describing a band crossing node at $k = b$ which may be understood as a Berry monopole [11–13] in the momentum space with non-trivial topological charge. Extensive theoretical studies have been performed for TSMs, including the topological quantum chemistry [14] and symmetry-based indicators theories [15–17], which provides a powerful tool for the high-throughout identifications of TSMs in non-magnetic crystalline materials [18–20], while the topological classifications and material realizations in magnetic phases are yet challenging [21, 22].

Besides the great achievements in the theoretical studies for TSMs, the unambiguous detection of their bulk band topologies still remains an urgent problem in this field. Usually in experiments, the detection of the bulk topological nodes relies on the measurements for the boundary modes due to the so-called bulk-boundary correspondence [23–28], which is an indirect detection method with ambiguities since usually the surface states depend on the surface terminations [29–32], which requires high qualities of the preparations and purifications of the materials, and also sometimes the topological surface states may merge with the trivial surface states, which gives difficulties for the distinguishement.

In this Letter, to attack on this question, we propose an novel approach for the detection of the bulk band crossing nodes of topological nodal systems without evolving any edge mode. The spirit of the here proposed method is to couple the system with an external field $A = a + A(X)$, which lives in a compact manifold with a spatial varying texture. The introduced field $A$ will bring a perturbation that leads to the variation of the wave vector $k$ of the targeted Hamiltonian $\hat{H}(k)$, meaning that for example we can transform the Weyl point model as $\hat{H}(k + A) = (k - b + A) \cdot \sigma$, then the system can have a response current $J$ as the conjugate field of $A$ which can be expressed as $J = \partial \hat{H} \over \partial A$. This process is like that we are enclosing the nodal point with the field $A$ in a compact manifold, and later we can see that for a nodal system the response current $J$ has a similar spatial texture as the applied field $A$ only when $A \rightarrow b$, which means we are hitting at the Berry monopole. Then we may turn the detection of the Berry monopole into the synthetic $J$ space to see if it shows a similar spatial texture of the $A$ field we use, and based on its spatial texture we may construct a Berry monopole indicator (BMI) $w$ [33, 34]. When $A$ goes close to the Berry monopole, the BMI $w$ may show a quantized fingerprint which can be expressed using the following limit:

$$\lim_{A \rightarrow b} w(A) \in \mathbb{Z}. \quad (1)$$

Thus the difference of the BMI $w$ between a quantized value gives a measure to the distance between the field $A$ to the Berry monopole $b$.

General framework.— We first expose the general framework of our proposal. In order to construct a general theory, we consider a $d$-dimensional system with a linear band crossing point at $k = b$, which locally can be described with the following model Hamiltonian:

$$\hat{H}(k) = \sum_{i=1}^{d} (k_i - b_i) \cdot \Gamma_i = (k - b) \cdot \Gamma, \quad (2)$$
while $\Gamma_i$ are $N = 2^n$ dimensional Dirac matrices satisfying the Clifford algebra as $\{ \Gamma_i, \Gamma_j \} = 2\delta_{ij}$. By applying a weak external field $A$, the Hamiltonian is perturbed and may be modified as:

$$\hat{H}(\mathbf{k} + A) = (\mathbf{k} - \mathbf{b} + A) \cdot \Gamma,$$

We require that the values of the $A$ field lives in a compact manifold with a spatial varying texture. Practically for a $d$-dimensional model we restrict $A$ on a $d$-sphere $S^d$ satisfying:

$$\sum_{i=1}^{d} (A_i - a_i)^2 = R^2,$$

with $a_i$ is the center and $R$ is the radius of the $S^d$ sphere. This applied field $A$ can give a variation of the wave vector $k$, we can define a response current $J$ as:

$$J = \frac{\partial \hat{H}(\mathbf{k} + A)}{\partial \mathbf{k}} = \Gamma.$$

The Matsubara Green function of Eq. (3) is:

$$\hat{G}(\varepsilon, \mathbf{k}, A) = \frac{1}{\varepsilon - \hat{H}(\mathbf{k} - \mathbf{b} + A)}.$$

Then the expectation value for $\langle J_i \rangle$ can be evaluated as:

$$\langle J_i \rangle = \text{Tr} \int \frac{d\mathbf{k} d\varepsilon}{(2\pi)^d(2\pi)} J_i \hat{G}(\varepsilon, \mathbf{k}, A)$$

$$= - \text{Tr} \int \frac{d\mathbf{k} d\varepsilon}{(2\pi)^d(2\pi)} \frac{\varepsilon + (\mathbf{k} - \mathbf{b} + A) \cdot \Gamma}{\varepsilon^2 + (\mathbf{k} - \mathbf{b} + A)^2} \Gamma_i$$

$$= - \int \frac{d\mathbf{k}}{(2\pi)^d} \frac{k_i - b_i + A_i}{\sqrt{\sum_{i=1}^{d} (k_i - b_i + A_i)^2}}.$$

The above approximations work well only when $(A_i - b_i) \to 0$, which requires that $a_i - b_i \to 0$ and $R \to 0$, meaning that the Berry monopole is enclosed by the $A$ with a compact manifold and the center of $A$ is hitting the Berry monopole, as shown in Fig. 1. By now the response current $J$ has the similar spatial texture as the external field $A$ which can be described with the following geometrical equation:

$$\sum_{i=1}^{d} \frac{(J_i - \alpha_i - b_i)^2}{\beta_i} = \sum_{i=1}^{d} (A_i - a_i)^2 = R^2.$$

Based on the spatial texture of $J$, the BMI $w$ can be defined. We illustrate this point by performing two case studies in two-dimensional (2D) and three-dimensional (3D). In different scenarios, the field $A$ and current $J$ can have different explanations. In the case studies, we restrict to Weyl point model formed by two spin polarized bands, in which the external field $A$ can be chosen as a Zeeman field $B$ and correspondingly the current $J$ is the magnetization $\mathcal{M}$, while our theory is general.

Weyl point in 2D. — Consider a Weyl point model in

![FIG. 2. The density plot of the distance function $d_2(B, \mathcal{B})$, which is peaked at $(B_1, B_2) = 0$ meaning that we are hitting the Berry monopole at $k = 0$.](image)
with \((B_1, B_2)\) is the center acting as an offset and \(R\) is the radius of the loop. We have the following current operator as:

\[
J = \left( \frac{\partial \hat{H}}{\partial k_x}, \frac{\partial \hat{H}}{\partial k_y} \right) = (\sigma_x, \sigma_y),
\]

(12)

which is just the magnetization \(\mathcal{M} = (\mathcal{M}_x, \mathcal{M}_y)\). From the previous discussions, when \((B_x, B_y)\) are small, the expectation values for the current \(J\) \((\langle \sigma_x \rangle, \langle \sigma_y \rangle)\) can be approximated as:

\[
\begin{align*}
\langle \sigma_x \rangle &= \alpha_1 + \beta_1 B_x, \\
\langle \sigma_y \rangle &= \alpha_2 + \beta_2 B_y,
\end{align*}
\]

(13)

with \((\alpha_1, \alpha_2)\) are offsets and \((\beta_1, \beta_2)\) are susceptibilities to the Zeeman field. Presently the current \(J\) has the same spatial texture as the Zeeman field \(B\), and we can have the following BMI \(w_2\) to be the vorticity of current \(J\) as:

\[
w_2 = \frac{1}{2\pi R^2} \int (dB_x, dB_y) (-\langle \sigma_y \rangle / \langle \sigma_x \rangle, \langle \sigma_x \rangle / \langle \sigma_x \rangle)
\]

\[
= \frac{1}{2\pi R^2} \int (dB_x, dB_y) (-\frac{\alpha_2}{\beta_2} - B_y, \frac{\alpha_1}{\beta_1} + B_x)
\]

\[
= \frac{1}{2\pi R^2} \int_0^{2\pi} d\alpha (-R \sin \alpha, R \cos \alpha) (-\frac{\alpha_2}{\beta_2} - B_y - R \sin \alpha, \frac{\alpha_1}{\beta_1} + B_x + R \cos \alpha)
\]

\[
= \frac{1}{2\pi R^2} \int_0^{2\pi} R^2 (\cos^2 \alpha + \sin^2 \alpha) d\alpha = 1,
\]

(14)

meaning that when the Zeeman field hits the Berry monopole, we have the following limit as:

\[
\lim_{\mathcal{B} \to 0} w_2 = 1.
\]

(15)

To confirm our proposal, we have carried out numerical investigations by putting Eq. (10) into a \(20 \times 20\) square lattice, for the discrete numerics the \(w_2\) can be expressed as:

\[
w_2 = \frac{1}{NR} \sum_i \left[ \sin \alpha_i \langle \sigma_y \rangle_i / \beta_2 + \cos \alpha_i \langle \sigma_x \rangle_i / \beta_1 \right]
\]

(16)

with the susceptibilities \(\beta_1\) and \(\beta_2\) can be evaluated step-wisely as:

\[
\beta_1 = \frac{\Delta \langle \sigma_x \rangle}{\Delta B_x}, \quad \beta_2 = \frac{\Delta \langle \sigma_y \rangle}{\Delta B_y}.
\]

(17)

In order to be minimal, we just need three measurements and pick up the angle \(\alpha\) to be set \(\alpha = 0, \frac{\pi}{4}, \text{and} \frac{3\pi}{4}\). We fix \(R = 0.001\) and modify \((B_1, B_2)\) to see the variation of \(w_2\). For the convenience of presentation, we define a distance function \(d(B_1, B_2) = \exp(-|w_2(B_1, B_2) - 1|)\) which characterizes the distance between the values of \(w_2\) and 1, and make a density plot as shown in Fig. 2. It is clearly seen that when \((B_1, B_2) = (0, 0)\) the distance function \(d(B_1, B_2)\) peaks at 1, indicating that we are exactly hitting at the Berry monopole, thus proving our proposal.

Weyl point in 3D. — Next we consider a Weyl point \(k = 0\) in 3D, which can be expressed as:

\[
\hat{H}(k) = k_x \sigma_x + k_y \sigma_y + k_z \sigma_z,
\]

(18)

the Pauli matrices \(\sigma_i\) \((i = x, y, z)\) acts on the spin space, thus the model Hamiltonian can describe a Weyl point in a 3D magnetic Weyl semimetal such as Co3Sn2S2 [29–32]. As in the 2D case, we can couple a Zeeman field \(\mathcal{B} = (B_x, B_y, B_z)\) to the model Hamiltonian as:

\[
\hat{H}(k) = (k_x + B_x) \sigma_x + (k_y + B_y) \sigma_y + (k_z + B_z) \sigma_z,
\]

(19)

The value of the Zeeman field \(\mathcal{B}\) now is restricted on a \(S^3\) sphere which may be expressed as:

\[
(B_x - B_1)^2 + (B_y - B_2)^2 + (B_z - B_3)^2 = R^2,
\]

(20)

with \((B_1, B_2, B_3)\) is the center and \(R\) is the radius. Similarly we can define the current \(J\) as:

\[
\mathbf{j} = \left( \frac{\partial \hat{H}}{\partial k_x}, \frac{\partial \hat{H}}{\partial k_y}, \frac{\partial \hat{H}}{\partial k_z} \right) = (\sigma_x, \sigma_y, \sigma_z),
\]

(21)

which maps to the 3D magnetization \(\mathcal{M} = (\mathcal{M}_x, \mathcal{M}_y, \mathcal{M}_z)\). Similarly the expectation values \(\langle \sigma_x \rangle, \langle \sigma_y \rangle, \text{and} \langle \sigma_z \rangle\) can be solved as:

\[
\begin{align*}
\langle \sigma_x \rangle &\approx \alpha_1 + \beta_1 B_x, \\
\langle \sigma_y \rangle &\approx \alpha_2 + \beta_2 B_y, \\
\langle \sigma_z \rangle &\approx \alpha_3 + \beta_3 B_z.
\end{align*}
\]

(22)

The above approximations work only if \(|\mathcal{B}| \to 0\), which requires \((B_1, B_2, B_3) \to 0\) and also \(R \to 0\), meaning that we also need to hit the Berry monopole. In the present case we can define the following Berry monopole indicator \(w_3\) as the flux of \(\mathbf{j}\) which can be expressed as:

\[
\text{(to be continued...)}
\]
we fix \( B_i = 0 \) and vary \((B_j, B_k)\) \((i,j,k=1,2,3)\) to see the variations of \( d_3 \) as shown in Fig. 3(a,b,c). It is clear that the distance function \( d_3 \) peaks at \((B_1, B_2, B_3) = 0\), showing that when we hit exactly at the Berry monopole, we can get the quantized value of \( w_3 \).

**Summary and Discussions.** — In summary, in this work we propose a new method for the detection of the band crossing points in topological nodal systems. The here proposed approach is to couple the targeted Hamiltonian with an external field \( \mathbf{A} \) in a compact manifold with spatial varying texture, which is like that we are enclosing a nodal point \( \mathbf{b} \) with \( \mathbf{A} \) which can generate a response current \( \mathbf{J} \). When \( \mathbf{A} \) hits the band crossing node, the current \( \mathbf{J} \) will show a similar spatial texture as the field \( \mathbf{A} \), then the detection of the topological node \( \mathbf{A} \) can be turned into the measurement of \( \mathbf{J} \)’s spatial texture thus a Berry monopole indicator can be constructed. Here we also point out that this proposed method is suitable for the detections of isolated band crossing nodes while the discussions for nodal line systems will appear in upcoming works. Our work has provided a novel method towards the unambiguous detection of the band topology of topological nodal systems and pave the way for further theoretical and experimental studies.

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