Merging of momentum-space monopoles by controlling magnetic field: From cubic-Dirac to triple-Weyl fermion systems

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We analyze a generalized Dirac system, where the dispersion along the \( k_x \) and \( k_y \) axes is \( N \)-th power and linear along the \( k_z \) axis. When we apply magnetic field, there emerge \( N \) monopole-antimonopole pairs beyond a certain critical field in general. As the direction of the magnetic field is rotated toward the \( z \) axis, monopoles move to the north pole while antimonopoles move to the south pole. When the magnetic field becomes parallel to the \( z \) axis, they merge into one monopole or one antimonopole whose monopole charge is \( \pm N \). The resultant system is a multiple-Weyl semimetal. Characteristic properties of such a system are that the anomalous Hall effect and the chiral anomaly are enhanced by \( N \) times and that \( N \) Fermi arcs appear. These phenomena will be observed experimentally in the cubic-Dirac and triple-Weyl fermion systems (\( N = 3 \)).

**Introduction:** Topological objects in the momentum space play intriguing roles in the field of condensed matter physics. Examples are monopoles, skyrmions and merons. They have fascinating properties that are not shared by the corresponding ones in the real space, since they are purely static because of the absence of the kinetic energy. For instance, a monopole carrying a large magnetic charge cannot exist in the real space due to a large Coulomb repulsion but can in the momentum space. It is an interesting problem if we may generate \( N \) monopole-antimonopole pairs and successively make them merged into one monopole-antimonopole pair each of which carries monopole charge \( \pm N \) just by controlling an external parameter.

Weyl semimetal is characterized by the monopole charge in the momentum space\(^{1,2} \). Characteristic features of Weyl semimetals are the emergence of the anomalous Hall conductance\(^{13,14} \), the chiral anomaly\(^{15,16} \) and the Fermi arc\(^{17,18} \). Double- and triple-Weyl semimetals are generalization of Weyl semimetals, where the monopole charges are 2 and 3, respectively\(^{19,20} \). It has theoretically been proposed that quadratic- and cubic-Dirac insulators are also possible based on the symmetry consideration\(^{21} \). The dispersion is parabolic or cubic along the \( k_x \) and \( k_y \) directions, while it is linear along the \( k_z \) direction. Very recently, it is shown that the cubic Dirac semimetals would be materialized in quasi-one-dimensional transition-metal monochalcogenides by first-principles calculations\(^{22} \).

In this paper we propose a simple model realizing a merging process of monopoles in the momentum space. It is a generalized Dirac system, where the dispersion along the \( k_x \) and \( k_y \) axes is \( N \)-th power and is linear along the \( k_z \) axis. Let us apply magnetic field. Unless its direction is not along the \( z \) axis, these Weyl fermions with the positive monopole charge move to the north pole, while those with the negative monopole charge move to the south pole. When the magnetic field approaches parallel to the \( z \) axis, they merge into one multiple-Weyl point whose monopole charge is \( N \). We show in such a system that the anomalous Hall effect and the chiral anomaly are enhanced by \( N \) times, and furthermore that \( N \) Fermi arcs emerge. These phenomena will be observed experimentally in the quadratic and cubic Dirac fermion systems.

**Model Hamiltonian:** We investigate the following Hamiltonian in the momentum space \((k_x, k_y, k_z)\),

\[
H = \tau_z \left[ \alpha a^N \left( k_x^N \sigma_+ + k_y^N \sigma_- \right) + t_z a_z k_z \sigma_z \right] + m \tau_x + \hbar \cdot \sigma, \tag{1}
\]

where \( N \) is an arbitrary natural number; \( k_{\pm} = k_x \pm ik_y; \) \( t, t_z \) are constants of energy dimension; \( a, a_z \) are constants of length dimension; \( m \) is the mass parameter taken in energy dimension \((m > 0)\); \( \hbar \cdot \sigma \) represents the Zeeman energy due to external magnetic field (let us call \( \hbar \) magnetic field); \( \sigma \) and \( \tau \) are the Pauli matrices describing the spin and pseudospin degrees of freedom, respectively; \( \sigma_\pm = \sigma_x \pm i\sigma_y \). For simplicity we set \( t = t_z = 1 \) in what follows. They can be easily recovered since they appear always in pairs with \( a \) and \( a_z \).

**Magnetic field:** When \( \hbar = 0 \), the Hamiltonian describes an insulator with massive Dirac electrons whose dispersion is \( N \)-th power along the \( k_x \) and \( k_y \) directions and linear along the \( k_z \) direction: See Fig\[\text{a}\]. Without loss of generality we can choose \( \hbar = h(\sin \theta, 0, \cos \theta) \) and \( h > 0 \). The Hamiltonian\(^{4} \) yields the energy spectrum \( E_{\chi \eta} = \chi \sqrt{F + 2\eta \hbar} \) with \( \chi = \pm 1, \eta = \pm 1, \) and

\[
F = (ak)^{2N} + \hbar^2 + m^2 + a_z^2 k_z^2, \tag{2}
\]

\[
G = m^2 + ((ak)^{N} \cos N \phi \sin \theta + a_z k_z \cos \theta)^2, \tag{3}
\]

where we have set \( k_x = k \cos \phi \) and \( k_y = k \sin \phi \). The gap is given by \( \Delta = \sqrt{m^2 - \hbar^2} \) at \( k = 0 \) for \( h < m \). As \( h \) increases the gap decreases and closes at the critical value \( h = m \), as shown in Fig\[\text{b}\]. Then, for \( h > m \), the band splits into \( N \) Weyl points and \( N \) anti-Weyl points with the linear dispersion, as shown in Fig\[\text{c}\]. The zero-energy solutions at these \( 2N \) points are given by

\[
ak_x = \left( h^2 - m^2 \right)^{1/2} \cos (j\pi/N) \sin \theta, \tag{4}
\]

\[
ak_y = \left( h^2 - m^2 \right)^{1/2} \sin (j\pi/N) \sin \theta, \tag{5}
\]

\[
ak_z = \pm \sqrt{h^2 - m^2} \cos \theta, \tag{6}
\]

with \( j = 1, \cdots, 2N \).

The Fermi surface is composed of the zero-energy points. All of them are on a single plane parallel to the \( k_x k_y \) plane at \( k_z \) fixed by \( (6) \). We show the almost zero-energy surface given
by $E = \delta$ for a fixed small value of $\delta$ at $h = 2m$ in Fig.2(a1) and (c1) for $N = 2$ and 3, respectively. Each of these points on the plane at $k_z > 0$ ($k_z < 0$) is a monopole (antimonopole) with the monopole charge $\pm 1$.

This can be seen in the standard way. Namely, we solve for the eigenstate $|\psi\rangle$ in the Hamiltonian (1), calculate the Berry connection by $A_i (k) = -i\langle \psi | \partial_i | \psi \rangle$ and the Berry curvature by $\Omega (k) = \nabla \times A (k)$, where $\partial_i = \partial / \partial k_i$. We show the Berry curvature at $h = 2m$ in Fig.2(b1) and (d1) for $N = 2$ and 3, respectively. Each Weyl (anti-Weyl) point has a hedgehog (anti-hedgehog) structure and possess the unit (minus unit) of monopole charge in the Berry curvature. The $N$ Weyl (anti-Weyl) points merge into one Weyl (anti-Weyl) point at $h = (0, 0, h)$. The coordinate of the point is given by $(0, 0, \pm \sqrt{h^2 - m^2})$, which we call the north or south pole. We clearly see how the $N$ hedgehog structures merge into one hedgehog structure in Fig.2. The dispersion along the $k_x$ and $k_y$ axes is the $N$-th power, which manifests that the Fermi surface is largely flattened along the $k_x$ and $k_y$ directions compared with the $k_z$ direction as shown in Fig.2(a5) and (c5).

Anomalous Hall effects: It is known that a pair of Weyl points contributes to the anomalous Hall conductance, which is proportional to the distance of the pair. It is due to the fact that the system has a nontrivial Chern number as a function of $k_z$. We seek whether similar phenomena exist in the present system.

The anomalous Hall conductance is given by $\sigma_{xy} = (e^2 / h)\varepsilon_{ij} \int C (k_t) dk_t$, where $C (k_t)$ is the Chern number at $k_t$ and defined by $C (k_t) = \sum_{\nu} C_{\nu} (k_t)$ with $C_{\nu} (k_t) = (1/2\pi)\varepsilon_{ij} \int dk_x dk_y \Omega_{\nu} (k)$. The summation $\sum_{\nu}$ runs over the occupied bands indexed by $\nu$. Here, $C_{\nu} (k_t)$ is the total Berry magnetic flux through the $k_t$ plane that comes from the band indexed by $\nu$.

A monopole charge is given by the surface integral of the Berry magnetic flux surrounding a Weyl point. We take a cylindrical surface containing a single Weyl point whose thickness is infinitesimally small and whose radius is infinite. Let the vector parallel to the cylindrical axis be $|\psi\rangle = (\sin \theta, 0, \cos \theta)$. We focus on the Chern number $C (k_\theta) = C (k_x) \sin \theta + C (k_z) \cos \theta$ with $k_\theta = k_x \sin \theta + k_z \cos \theta$. The contribution from the side of the cylinder is zero. The contribution from the top and bottom surfaces are the Chern numbers $C (k_\theta + \delta)$ and $C (k_\theta - \delta)$, respectively, and hence the total contribution is $C (k_\theta + \delta) - C (k_\theta - \delta) = \pm 1$ for a monopole or an antimonopole. Since there are no monopoles and no antimonopoles as $k_\omega \to -\infty$, we set $\lim_{k_\omega \to -\infty} C (k_\theta) = 0$. In this way $C (k_\theta)$ is obtained as a function of $k_\theta$.

The Chern number $C (k_z)$ is calculated as follows. For the band with $\chi = -1$ and $\eta = 1$, we obtain explicitly as

$$C_{\nu} (k_z) = \begin{cases} N/2 & \text{for } a_\nu |k_z| > \sqrt{h^2 - m^2} \cos \theta \\ -N/2 & \text{for } a_\nu |k_z| < \sqrt{h^2 - m^2} \cos \theta \end{cases}.$$ (7)

It changes the sign at the position of the Weyl and anti-Weyl points. On the other hand, the Chern number does not change as a function of $k_z$ for the band with $\chi = -1$ and $\eta = 1$, $C_{\nu} (k_z) = -N/2$. The total Chern number is given by the sum of these two contributions and given by

$$C (k_z) = \begin{cases} 0 & \text{for } a_\nu |k_z| > \sqrt{h^2 - m^2} \cos \theta \\ -N & \text{for } a_\nu |k_z| < \sqrt{h^2 - m^2} \cos \theta \end{cases}.$$ (8)

Similarly we can calculate $C (k_x)$ and $C (k_y)$.

It follows that the anomalous Hall conductance is given as

$$\sigma_{xy} = N \frac{e^2}{\pi h} \sqrt{h^2 - m^2} \cos \theta.$$ (9)

It is enhanced by $N$ times compared with that in normal Weyl semimetals.

Fermi arcs: In what follows we study the case $h = (0, 0, h)$. $N$ Weyl points merge into a single multiple-Weyl point at the north or south pole for $h > m$. To such a case we apply the same argument and find that the monopole charge at the north (south pole) is $\pm N$. The system is a quantum anomalous Hall insulator for each $k_z$ when $a_\nu |k_z| < \sqrt{h^2 - m^2}$. The $N$ chiral edge modes appear at the sample edges based on the bulk-edge correspondence. Each chiral edge must cross the Fermi energy at a certain momentum $k_\omega$.

Multiple-Weyl fermions: In order to make a further study of the monopole, we derive the effective Hamiltonian for multiple-Weyl fermions under the magnetic field $h = (0, 0, h)$ with $h > m$. We first construct a unitary transformation $U$ that diagonalizes the Hamiltonian $H (0, 0, k_z)$. We then transform the Hamiltonian $H (k_x, k_y, k_z)$ by the same unitary transformation $U$.
transformation $U$. We may extract the $2 \times 2$ matrix whose eigenvalues vanish at the north and south poles. Expanding it around $k_z = \pm \sqrt{\hbar^2 - m^2}$, we obtain

$$
H_{\text{eff}} = -a^N (k_+^N \sigma_- + k_-^N \sigma_+) + \frac{m^2}{\hbar^2} \left( a_z k_z \mp \sqrt{\hbar^2 - m^2} \right) \sigma_z.
$$

(10)

This is the effective Hamiltonian valid around the north or south pole.

We prove that the north pole has the monopole charge $N$. With the use of the eigenstate of the Hamiltonian $| \Omega \rangle$ we may derive the Berry curvature as

$$
(\Omega_x, \Omega_y, \Omega_z) = \frac{N a^{2N} a_z \left( k_x^2 + k_y^2 \right)^{N-1} (k_x, k_y, Nk_z)}{2 \left( a^N (k_x^2 + k_y^2)^N + a_z^2 k_z^2 \right)^{3/2}}.
$$

(11)

This describes the momentum-space monopole at the north pole. It is easy to show $\partial_i \Omega_i(k) = 0$ except for $k = 0$. Hence, we find $\partial_i \Omega_i = \rho \delta(k)$ with a constant $\rho$. We make a change of the variables, $k_x = (K \sin \theta)^{1/N} \cos \phi$, $k_y = (K \sin \theta)^{1/N} \sin \phi$ and $k_z = K \cos \theta$, with $(K, \theta, \phi)$ being the polar coordinate. To determine the constant $\rho$, we use the Gauss theorem by choosing a sphere with radius $K$. We then
have
\[ \rho = \epsilon_{ij\ell} \int \Omega_i dk_j dk_l = \frac{N}{2} \int \sin \theta d\theta d\phi = N \quad (12) \]
after a straightforward calculation.

**Landau levels:** When the magnetic field is strong enough, the cyclotron motion in the \( xy \) plane forms Landau levels. As a result, the system becomes a one-dimensional system along the \( k_z \) axis. By making the minimal substitution, the Hamiltonian is given by
\[ H = z \left( \hbar \omega_c \hat{a}^\dagger \right)^N \sigma_- + \hbar \omega_c \hat{a}^N \sigma_+ + a_z k_z \sigma_z + m \tau_x, \quad (13) \]
where \( \hat{a} \) is the Landau-level ladder operator with \( [\hat{a}, \hat{a}^\dagger] = 1 \), and \( \hbar \omega_c \) is the cyclotron energy. The bulk spectrum is obtained,
\[ E_{N}^{\chi \eta} = \chi \sqrt{\frac{(n + N)!}{n!}} \hbar \omega_c + \left( \sqrt{a_z^2 k_z^2 + m^2 + \eta \hbar} \right), \quad (14) \]
with the eigenstates being
\[ \psi = (u_n |n\rangle, u_{n+N} |n+N\rangle, u_{n} |n\rangle, u_{n+N} |n+N\rangle)^T, \quad (15) \]
for \( n = 0, 1, 2, \ldots \). In addition we have \( N \)-fold degenerated Landau levels
\[ E = -\hbar \pm \sqrt{a_z^2 k_z^2 + m^2}, \quad (16) \]
with the eigenstates being \( \psi = (0, u_{\nu} |\nu\rangle, 0, u_{\nu} |\nu\rangle)^T \), where \( \nu = 0, \ldots, N-1 \). We show the Landau levels as a function of \( k_z \) in Fig.3 Chiral edge modes emerge for \( |h| > m \), where the degeneracy is \( N \). Hence, the chiral anomaly is enhanced by \( N \) times.

**Lattice Hamiltonian:** It would be interesting to construct a lattice Hamiltonian, from which the continuum Hamiltonian follows as a low energy theory. A simplest realization would be
\[ H = -2^{N-1} \tau_z \left[ \sigma_z \prod_{j=1}^{N} \sin (d_j^1 \cdot k) + \sigma_\sigma \prod_{j=1}^{N} \sin (d_j^2 \cdot k) \right] + t_z \sigma_z \sin a_z k_z + m \tau_x + h \cdot \sigma, \quad (17) \]
with \( d_j^1 = a (\sin [(2j + 1) \pi/2N], \cos [(2j + 1) \pi/2N], 0) \) and \( d_j^2 = a (\sin [j \pi/N], \cos [j \pi/N], 0) \), where \( t, t_z \) are transfer energies, and \( a, a_z \) are lattice constants. The energy spectrum has the zero-energy points at the \( \Gamma \) point \((0, 0, 0)\). In the vicinity of the \( \Gamma \) point, the lattice Hamiltonian is expanded and yields the continuum Hamiltonian.

**Discussions:** We have studied a merging process of \( N \) monopoles into one monopole carrying monopole charge \( N \) based on the continuum Hamiltonian. We have constructed a lattice Hamiltonian from which the continuum Hamiltonian is derived. In the lattice Hamiltonian, \( N \) represents the number of the nearest adjacent sites. Hence, the case for \( N = 2 \) can be embedded into the layered square lattice, while the case for \( N = 3 \) can be embedded into the layered triangular lattice. On the other hand, it is impossible to embed the cases for \( N \geq 4 \) into the realistic lattice as far as we employ this lattice Hamiltonian.

Finally we would argue a possible experimental study of the merging process. When the mass parameter \( m \) is large the magnetic field becomes too large to carry out any experiments. However, our theory is valid however small \( m \) may be. Recent study shows that a cubic-Dirac semimetal is realized in quasi-one-dimensional transition-metal monochalcogenides by first-principles calculations, where the mass parameter is almost zero. It is easy to realize the topological phase transition for small \( m \) since the transition occurs at \( h = m \). In this sense, quasi-one-dimensional transition-metal monochalcogenides will be an ideal playground to verify the results in our predictions.

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