Magnonic Weyl semimetal in pyrochlore ferromagnets

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Topological states of matter have been a subject of intensive studies in recent years because of their exotic properties such as the topologically protected edge and surface states. The initial studies were exclusively for electron systems. It is now known that topological states can also exist for other particles. Indeed, topologically protected edge states have already been found for phonons and photons. In spite of active searching for topological states in many fields, the studies in magnetism are relatively rare although topological states are apparently important and useful in magnonics. Here we show that the pyrochlore ferromagnets with the Dzyaloshinskii-Moriya interaction are intrinsic magnonic Weyl semimetals. Similar to the electronic Weyl semimetals, the magnon bands in a magnonic Weyl semimetal are nontrivially crossing in pairs at special points (called Weyl nodes) in momentum space. The equal energy contour around the Weyl nodes gives rise to the Fermi arcs on sample surfaces due to the topologically protected surface states between each pair of Weyl nodes. Additional Weyl nodes and Fermi arcs can be generated in lower energy magnon bands when an anisotropic exchange interaction is introduced.

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I. INTRODUCTION

Magnetic materials are highly correlated spin systems that do not respect time-reversal symmetry. Their static states, such as domains, domain walls, and skyrmions, are the energy minimum spatial configurations of magnetization (vector order parameter). The excitations of magnetic materials are spin waves whose quanta are magnons of spin-1 particles. Like electrons, magnons can carry, process and transmit information besides being a control knob of magnetization dynamics. In fact, magnonics is a very active research field because of low energy consumption of magnonic devices and possible long spin coherence length. One important issue in magnonics is the efficient transportation of magnons. Magnon (spin wave) flux normally decays fast during its propagation because it is difficult to confine magnons in the space. Finding materials or structures that can confine the motion of magnons in a restricted region under topological protection should open doors to new functional devices. Thus, the realization of topological states of matter in magnetic systems should be highly desirable.

In this work, we show that the pyrochlore ferromagnet Lu\textsubscript{2}V\textsubscript{2}O\textsubscript{7}, which was recently shown to exhibit magnon Hall effect, is an intrinsic magnonic Weyl semimetal (MWS). Two adjacent magnon bands in a MWS nontrivially cross each other at some special points called Weyl nodes (WNs) in momentum space. The WNs are monopoles of Berry curvature and are characterized by integer topological charges. Because the net topological charges in the entire Brillouin zone (BZ) must be zero, the WNs must appear in pairs with opposite topological charges. Like the electronic Weyl semimetal, the MWS has topologically protected chiral surface states between each pair of WNs on the sample surfaces. The equal energy contour of these surface states form arcs (called Fermi arc), and the number of Fermi arcs between two paired WNs equals to the number of topological charges carried by one of them. Moreover, additional WNs and topologically protected surface states can appear in lower energy magnon bands when anisotropic exchange interaction, possibly induced by either doping or strain along the [111] direction, is introduced.

II. RESULTS

A. The effective spin model of Lu\textsubscript{2}V\textsubscript{2}O\textsubscript{7}

Lu\textsubscript{2}V\textsubscript{2}O\textsubscript{7} is an intrinsic ferromagnetic Mott-insulator in which each vanadium ion V\textsuperscript{4+} carries spin $S = 1/2$. The magnetic properties of the material come purely from the vanadium ions that form a pyrochlore lattice consisting of four interpenetrating face-centered cubic (FCC) lattices with corner-sharing tetrahedrons, as shown in Fig. 1a. The primitive vectors are $a_1 = (1,1,0)/2$, $a_2 = (1,0,1)/2$, and $a_3 = (0,1,1)/2$, where the FCC lattice constant is set to unit. Three of the four FCC lattices are shifted by $a_1/2$, $a_2/2$, and $a_3/2$, respectively. In each unit cell, there are four V\textsuperscript{4+} ions as shown in Fig. 1b. Under an external magnetic field, the magnetic properties of the material is well described by a simple Heisenberg Hamiltonian with the Dzyaloshinskii-Moriya interaction (DMI). The effective spin Hamiltonian reads

$$H = -\sum_{\langle ij \rangle} J_{ij} \mathbf{S}_i \cdot \mathbf{S}_j + \sum_{\langle ij \rangle} D_{ij} (\mathbf{S}_i \times \mathbf{S}_j) - g\mu_B \sum_i \mathbf{h} \cdot \mathbf{S}_i,$$

where $\langle ij \rangle$ denotes the nearest neighbor (NN) sites and $\mathbf{S}_i$ is the spin of the V\textsuperscript{4+} ion at site $i$. $\mathbf{h}$ is the external field.
FIG. 1: (a) The pyrochlore structure of four interpenetrating face-centered cubic lattices with corner-sharing tetrahedrons. The orange dots denote the V$^{4+}$ ions. (b) The DMI vector configuration of a tetrahedron lying in a corner-sharing cubic. The arrows represent the DMI vectors $D_{ij}$ perpendicular to the bonds of the tetrahedron and parallel to the surfaces of the cubic. (c) The first bulk Brillouin zone (BZ) and the first (001) surface BZ of the pyrochlore lattice. The projection of the high symmetry points of the bulk BZ onto the surface BZ are denoted by the barred symbols. The red and blue dots schematically represent the pair of WNs with opposite topological charges between $E_2$ and $E_3$ bands. (d) The magnon energy spectrum along the high symmetry path shown in (c) with DMI (red curves) and without DMI (blue curves). (e) The magnon dispersion around the WN shown in (d) in the $k_z$-$k_d$ plane which is represented by the yellow plane in (c).

As it was explained in ref. [19], the material is a collinear ferromagnet in spite of the DMI because the summation of six DMI vectors adjacent to each lattice site is zero. Under the Holstein-Primakoff transformation and by using the Bloch theorem, the Hamiltonian (1) is block diagonalized in momentum space as

$$H(k) = \sum_k b_k^\dagger \mathcal{H}(k) b_k + E_0,$$

where $b_k = \left(b_{k,0}^\dagger, b_{k,1}^\dagger, b_{k,2}^\dagger, b_{k,3}^\dagger\right)$ and $b_k$ are the creation and annihilation operators of magnons (see Methods). The four components correspond to the four different FCC sublattices. $E_0 = -Ng\mu_B |h|/2 - \sum_{j \in \langle ij \rangle} J_{ij}/8$ is the energy of zero magnon state (vacuum), where $N$ is the total number of lattice sites and $j \in \langle ij \rangle$ denotes $j$ as the NN site of $i$ (see Methods). One can set $E_0$ to zero by choosing a proper energy reference. For a given $k$, $\mathcal{H}(k)$ is a $4 \times 4$ matrix

$$\mathcal{H}(k) = \begin{pmatrix} 3J & JA_1(k) & JA_2(k) & JA_3(k) \\ JA_1(k) & 3J & J-A_{12}(k) & J-A_{13}(k) \\ JA_2(k) & J+A_{12}(k) & 3J & J-A_{23}(k) \\ JA_3(k) & J-A_{13}(k) & J+A_{23}(k) & 3J \end{pmatrix},$$

where $A_{\alpha}(k) = -\cos(a_\alpha \cdot k/2)$, $A_{\alpha\beta}(k) = -\cos[(a_\alpha - a_\beta) \cdot k/2]$, and $J_{ij} = J$ for isotropic exchange interaction. The strength of the DMI is a constant $D = |D_{ij}|$. Because only the components of $D_{ij}$ parallel to the external magnetic field contribute to Hamiltonian (1) (see Methods), $J_k = J \pm i\sqrt{2}D/\sqrt{3}$ for $h$ along the [111] direction.[19] The magnitude of magnetic field is set as $|h| = 0^+$ for simplicity (and without loss of generality) since the Zeeman interaction only shifts the magnon dispersion relation and does not affect the topological properties. In the absence of DMI $D = 0$, the magnon spectrum contains two degenerate flat bands $E_i(k) = 4J$ ($i = 1,2$) and two dispersive
bands $E_i(k) = 2J \pm J \sqrt{1 + F(k)}$ ($i = 3, 4$), where $F(k) = \cos(k_x/2) \cos(k_y/2) + \cos(k_z/2) \cos(k_y/2) + \cos(k_y/2) \cos(k_z/2)$. The magnon dispersion relation along the high symmetry path $\Gamma$-K-W-X-U-$L$-$\Gamma$ (see Fig. 1) is shown in Fig. 1 for $D = 0$ (blue curves) and for the experimental value $D = 0.18 J$ (red curves). In comparison with the case of $D = 0$, the flat bands become dispersive and band gaps are opened.

**B. Identification of Weyl nodes and Fermi arcs**

Interestingly, a pair of WNs appears on the high symmetry line $L$-$\Gamma$-$L$ as shown in Figs 1c and 1d. Two magnon bands of $E_2$ and $E_3$ linearly cross each other, giving rise to a MWS behavior. Along the $L$-$\Gamma$-$L$ line, where $k = k_1(1, 1, 1)$, two magnon bands are flat with $E_i(k) = 4J \pm \sqrt{2}D$ ($i = 1, 2$), and the other two bands are dispersive with $E_i(k) = 2J \pm J \sqrt{2.5 + 1.5 \cos k_1}$ ($i = 3, 4$). For $D = 0$, $E_3$ touches $E_1$ and $E_2$ at the $\Gamma$ point. For modest $D > 0$, $E_1$ and $E_2$ are split into two nondegenerate flat bands, and $E_2$ and $E_3$ cross at a pair of WNs at

$$k_1 = \pm \cos^{-1} \left[ \frac{2(2J - \sqrt{2}D)^2 - 5J^2}{3J^2} \right].$$  (3)

$k_1 = \pm 1.198$ for $D = 0.18J$. Moreover, the flatness of $E_2$ along the $L$-$\Gamma$-$L$ line means the magnon group velocity near the WNs vanishes along the $[111]$ direction. According to a recent classification, this corresponds to the transition state from type-I to type-II Weyl semimetals with vanishing group velocity only in one direction. To visualize the magnon dispersion with vanishing group velocity only in one direction, we plot the magnon bands of $E_2$ and $E_3$ near one WN in a vertical plane (represented by the yellow plane in Fig. 1c) parallel to both $k_2$ direction and the diagonal $k_x$-$k_y$ direction (termed as $k_d$). Obviously, the $L$-$\Gamma$-$L$ line lies in the $k_x$-$k_y$ plane, and $E_2$ band and $E_3$ band linearly cross each other at the WN of $k = 1.198(1, 1, 1)$ as shown in Fig. 1e.

Similar to the electronic Weyl semimetal, one fingerprint of the MWS is the Fermi arcs on the sample surfaces. In order to illustrate this feature, we consider a slab whose surfaces are perpendicular to the $[001]$ direction. The first BZ of the (001) surface is shown in Fig. 1f, where the projection of the high symmetry points of the first bulk BZ onto the first surface BZ are denoted by the barred symbols. The pair of WNs are schematically represented by the red and blue dots (indicating they carry opposite topological charges) in Fig. 1f. The density plot of magnon spectral function on the top surface along the high symmetry path of $\Gamma$-$X$-$L$-$\Gamma$ is shown in Fig. 2a where one WN can be identified. The topologically protected surface states with high density on the top surface are represented by red color. On the path of $\Gamma$-$L$-$\Gamma$ where both of the two WNs lies in, the density plot of magnon spectral function on the top surface is shown in Fig. 2b. Apparently, the pair of WNs are connected by surface states. For fixed energies of $E_c$, $E_d$, and $E_e$ around the WNs (see Fig. 2b), the corresponding density plot of magnon spectral function on the top surface in the first BZ for fixed energies of $E_c$, $E_d$, and $E_e$ denoted in (a).

**C. Anisotropic exchange interaction**

We have shown that the pyrochlore ferromagnet Lu$_2$V$_2$O$_7$ is an intrinsic MWS. We would like to show now that more pairs of WNs and topologically protected surface states can come from the lower energy magnon bands of $E_3$ and $E_4$ in the presence of anisotropic exchange interaction. The pyrochlore lattice can be viewed as an alternative stack of Kagome and triangular lattices.
J can close the gap at the X point whenever shown in Fig. 1d. The anisotropic exchange interaction minimum between $E_t$ on each particular site is the sum of the exchange sublattice on-site potential because the one-site potential $E$ of the pyrochlore lattice. The red and blue dots schematically represent the three pairs of WNs with opposite topological charges between the bands of $E_3$ and $E_4$. The density plot of magnon spectral function on the top surface for $J' = J$ along the path of $\Gamma - \mathbf{K} - \mathbf{M} - \Gamma$. The density plot of magnon spectral function on the top surface for $J' = 0.6J$ along the paths of $\Gamma - \mathbf{K} - \mathbf{M} - \Gamma$ (upper panel) and $\Gamma - \mathbf{M} - \mathbf{M} - \Gamma$ (lower panel) that are presented by red solid and dash lines in (b). (e) The density plot of magnon spectral function on the top surface for $J' = 1.6J$ along the paths of $\Gamma - \mathbf{K} - \mathbf{M} - \Gamma$ (upper panel) and $\Gamma - \mathbf{M} - \mathbf{M} - \Gamma$ (lower panel) that are presented by blue solid and dash lines in (b). (f)-(g) The Fermi arcs on the top (111) surface for energies through the WNs for $J' = 0.6J < J'_c$ (f) and $J' = 1.6J > J'_c$ (g). The black hexagon encloses the first BZ.

along the [111] direction. In principle, the interlayer exchange interaction $J'$ differs from the intralayer exchange interaction $J$. $J'$ can be tuned by either doping or strain. The effective Hamiltonian with the anisotropic exchange interaction, under the same considerations as before, becomes

$$\mathcal{H}'(\mathbf{k}) = \begin{pmatrix}
3J' & J'A_1(\mathbf{k}) & J'A_2(\mathbf{k}) & J'A_3(\mathbf{k}) \\
J'A_1(\mathbf{k}) & 2J' + J & J_+A_{12}(\mathbf{k}) & J_+A_{13}(\mathbf{k}) \\
J'A_2(\mathbf{k}) & J_+A_{12}(\mathbf{k}) & 2J' + J & J_+A_{23}(\mathbf{k}) \\
J'A_3(\mathbf{k}) & J_+A_{13}(\mathbf{k}) & J_+A_{23}(\mathbf{k}) & 2J' + J'
\end{pmatrix}. \tag{4}$$

The anisotropic exchange interaction leads to different sublattice on-site potential because the one-site potential on each particular site is the sum of the exchange interaction strengths of all its NNS (see Methods).

For the isotropic exchange interaction, the energy gap minimum between $E_3$ and $E_4$ bands is at the X point as shown in Fig. 1d. The anisotropic exchange interaction can close the gap at the X point whenever $J'$ equals to two critical values

$$J'_\pm = \alpha \pm \sqrt{2\alpha^2 - 2\alpha J}, \tag{5}$$

where $\alpha = \sqrt{J'^2 + 2D^2/3}$. The critical $J'_\pm$ as functions of the DMI strength $D$ are plotted as red and blue curves in Fig. 3a. These are the phase boundaries between the normal magnonic insulator (without topologically protected surface states in the gap) and the MWS from $E_3$ and $E_4$ bands. The phase diagram of the MWS from $E_3$ and $E_4$ bands in the $D-J'$ plane is shown in Fig. 3a. In the shadowed regions of Fig. 3a, where $J' > J'_+$ or $J'_- > J' > 0$, $E_3$ and $E_4$ bands always cross at three pairs of WNs due to the three-fold rotation symmetry with respect to the L-$\Gamma$-L line (see Fig. 3a). For Lu$_2$V$_2$O$_7$, $J'_+ = 1.158J$ and $J'_- = 0.863J$. In the limits of $J' \to \infty$ and 0, all these WNs will merge at the L point. The fact that the trivial region represented by white color shrinks as $D$ decreases means that weak DMI is favorable for the existence of WNs between $E_3$ and $E_4$ bands since only weak anisotropy (small difference between the interlayer and intralayer exchange...
interactions) is required. These results are applicable to other pyrochlore ferromagnets.

D. Additional Weyl nodes and Fermi arcs

To visualize these additional WNs and topologically protected surface states existing in the MWS phase from \( E_3 \) and \( E_4 \) bands, the magnon spectral function of a slab with \((111)\) surfaces is calculated. The density plot of magnon spectral function on the top surface for \( J' = J \) along the high symmetry path \( \Gamma-K-M-\Gamma \) (marked by red solid lines in Fig. 3f) is shown in Fig. 3f. The energy gap minimum appears at the \( M \) point to which the \( X \) point is projected. As the interlayer exchange interaction decreases to \( J' = 0.6J < J'_c \), three pairs of WNs are created from the linear crossing of \( E_3 \) and \( E_4 \) bands. The density plot of magnon spectral function on the top surface in Fig. 3b) is shown in Fig. 3f. Along the path of \( \Gamma-K-M-\Gamma \), a WN is identified on the \( M-\Gamma \) segment. The topologically protected surface states is clearly visible within the energy gap with one end terminated at the WN. Along the path of \( \Gamma-M'-M-\Gamma \) (represented by red dash lines in Fig. 3f), a pair of WNs is connected by the surface states. Similar results for \( J' = 1.6J > J'_c \) are shown in Fig. 3f along the \( \Gamma-K'-M-M-\Gamma \) and \( \Gamma-M-M'-\Gamma \) paths (marked by blue solid and dash lines, respectively, in Fig. 3f). In order to detect the Fermi arc feature, we fix the energy through the WNs for the two different interlayer exchange interaction strengths. The density plot of magnon spectral function on the top surface in the two-dimensional momentum space is shown in Figs 3f and 3k where the black hexagon encloses the first surface BZ. Apparently, the topologically protected surface states form three Fermi arcs of three pairs of WNs.

The pair of WNs from \( E_2 \) and \( E_3 \) bands on the L-\( \Gamma-L \) line can remain for the anisotropic exchange interaction.

Three additional pairs of WNs can be generated from the linear crossing of \( E_2 \) and \( E_3 \) bands on the \( L-\Gamma-L \) line in momentum space. The distance between the paired WNs is determined by the strength of DMI. Similar to its electronic counterpart, the MWS has topologically protected chiral surface states whose equal energy contour yields the Fermi arc that connects the pair of WNs on the sample surfaces. By introducing different interlayer and intralayer exchange interaction strengths through either doping or strain along the \([111]\) direction, three additional pairs of WNs can be generated from the lower energy magnon bands of \( E_3 \) and \( E_4 \). On the surfaces of a slab perpendicular to the \([111]\) direction, the three pairs of WNs are connected by three Fermi arcs in two-dimensional momentum space. Furthermore, the pair of WNs between \( E_2 \) and \( E_3 \) bands can remain on the L-\( \Gamma-L \) line whose distance is determined by both the DMI and interlayer exchange interaction. These results are applicable to other collinear pyrochlore ferromagnets with anisotropic exchange interaction.

The MWS featured by WNs and Fermi arcs can be detected by inelastic neutron scattering which has been used to probe the magnon bands of a topological magnon insulator. The topologically protected magnon surface states can also be probed by the spin-polarized scanning tunneling microscopy through the second-order derivative of tunneling current that contains the information of electron-magnon scattering.

IV. METHODS

A. Holstein-Primakoff transformation

In this transformation, the spin-1/2 operators are mapped to the magnon creation and annihilation operators as

\[
S_i^+ = \sqrt{1-n_i}b_i, \quad S_i^- = b_i^\dagger\sqrt{1-n_i}, \quad n_i = b_i^\dagger b_i, \quad (7)
\]

where the ladder operators \( S_i^\pm = S_i^0 \pm iS_i^m \) are defined in the orthonormal coordinate \((l, m, n)\) with \( n \) axis parallel to the external magnetic field. For the DMI, the local spin \( S_i = S + \delta S_i \) where \( S = (0, 0, 1/2) \) and \( \delta S_i = (S_i^0, S_i^m, 0) \) in the linear approximation. Thus, the Hamiltonian of DMI is

\[
H_{DMI} = \sum_{(ij)} D_{ij} \cdot (S \times \delta S_j + \delta S_i \times S + \delta S_i \times \delta S_j)
\]

\[
= \sum_{(ij)} D_{ij} \cdot (0, 0, S_i^0 S_j^m - S_i^m S_j^0) \quad (8)
\]

\[
= \sum_{(ij)} \frac{iD_{ij}^n}{2} (S_i^+ S_j^- - S_i^- S_j^+) ,
\]

where \( D_{ij}^n = D_{ij} \cdot \hat{n} \) and \( \sum_{(ij)} D_{ij} \cdot (S \times \delta S_j + \delta S_i \times S) = 0 \). Namely, the \( D_{ij} \) with vanishing \( n \) component does

III. DISCUSSION

The pyrochlore ferromagnet Lu\(_2\)V\(_2\)O\(_7\) is an intrinsic topological material (called MWS) in the sense that two adjacent magnon bulk bands of \( E_2 \) and \( E_3 \) linearly cross each other at a special pair of points (called WNs) on the L-\( \Gamma-L \) line in momentum space. The distance between the paired WNs is determined by the strength of DMI. Similar to its electronic counterpart, the MWS has topologically protected chiral surface states whose equal energy contour yields the Fermi arc that connects the pair of WNs on the sample surfaces. By introducing different interlayer and intralayer exchange interaction strengths through either doping or strain along the \([111]\) direction, three additional pairs of WNs can be generated from the lower energy magnon bands of \( E_3 \) and \( E_4 \). On the surfaces of a slab perpendicular to the \([111]\) direction, the three pairs of WNs are connected by three Fermi arcs in two-dimensional momentum space. Furthermore, the pair of WNs between \( E_2 \) and \( E_3 \) bands can remain on the L-\( \Gamma-L \) line whose distance is determined by both the DMI and interlayer exchange interaction. These results are applicable to other collinear pyrochlore ferromagnets with anisotropic exchange interaction.
not contribute to the Hamiltonian. Substitute these into the effective spin Hamiltonian \([1]\), we get a tight-binding Hamiltonian of magnons as

\[
H = -\frac{1}{2} \sum_{\langle ij \rangle} \left[ (J_{ij} + iD_{ij}^b) b_i^\dagger b_j + \text{H.c.} \right] + E_0,
\]

\[
+ \sum_i \left( \sum_{j \in \langle i \rangle} \frac{J_{ij}}{2} + g\mu_B|\hbar| \right) b_i^\dagger b_i.
\]

Here \(j \in \langle i \rangle\) denotes \(j\) as the NN site of \(i\), and \(E_0 = -Ng\mu_B|\hbar|/2 - \sum_i \sum_{j \in \langle i \rangle} J_{ij}/8\) can be set to zero by choosing a proper energy reference, where \(N\) is the total number of lattice sites. Moreover, the on-site potential of each lattice site is determined by the sum of all adjacent NN exchange interaction strengths such that the anisotropic exchange interaction can generate different sublattice on-site potential as shown in equation \([4]\).

According to the Bloch theorem, the Hamiltonian \([4]\) is block diagonalized in the basis of Bloch states

\[
|k, \alpha \rangle = \frac{1}{\sqrt{N/4}} \sum_i e^{i\mathbf{k} \cdot \mathbf{r}_i} |i, \alpha \rangle,
\]

where \(\alpha = 0, 1, 2, 3\) denote four different sublattices shown in Fig. \([7]\), and \(\mathbf{r}_i\) is the position of the \(i\)th unit cell. Thus, we obtain the Hamiltonian \([2]\) and \([4]\).

### B. Surface spectral function.

The spectral function of a specific layer is

\[
A_l(k, E) = -\frac{1}{\pi} \text{Im} \left[ \text{Tr} G_{ll}(E, \mathbf{k}) \right],
\]

where \(l\) is the layer index and \(G_{ll}(E, \mathbf{k}) = \langle l| (E + i0^+ - H)^{-1} |l \rangle\). For the top surface with \(l = 1\), \(G_{11}(E, \mathbf{k})\) is obtained by the recursive Green’s function method\([30,31]\).

**Note added.** Upon completion of this work, we became aware of ref. \([32]\) in which part of the results were obtained.

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