Weyl-triplons in $\text{SrCu}_2(\text{BO}_3)_2$

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Weyl-triplons in $\text{SrCu}_2(\text{BO}_3)_2$

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We propose that Weyl triplons are expected to appear in the low energy magnetic excitations in the canonical Shastry-Sutherland compound, $\text{SrCu}_2(\text{BO}_3)_2$, a quasi-2D quantum magnet. Our results show that when a minimal, realistic inter-layer coupling is added to the well-established microscopic model describing the excitation spectrum of the individual layers, the Dirac points that appears in the zero-field triplon spectrum of the 2D model splits into two pairs of Weyl points along the k_z direction. Varying the strength of the inter-layer DM interaction and applying a small longitudinal magnetic field results in a range of band topology transitions accompanied by changing numbers of Weyl points. We propose inelastic neutron scattering along with thermal Hall effect as the experimental techniques to detect the presence of Weyl-node in the triplon spectrum of this material.

I. INTRODUCTION

The successful detection of Weyl fermions in TaAs[24], following theoretical prediction of the same[11, 53], marks one of the latest milestones in the study of topological phases of matter, currently the most active frontier in Condensed Matter Physics[1, 2, 19, 20, 46, 51, 52, 56, 57]. Weyl fermions are massless, linearly dispersing quasi-particles with finite chirality, first proposed as solutions to massless Dirac equation in relativistic particle physics[54]. Pairs of Weyl fermions with opposite chirality may combine to form Dirac fermion. In condensed matter systems, non-relativistic analog of Weyl quasi-particles emerge at linear crossing of non-degenerate, topologically protected bands in three dimensional reciprocal space. Interest in these special band crossings have increased since they act as sources of Berry flux and impart topological character to the associated energy bands. Weyl nodes appear in pairs with opposite chirality and can be separated in momentum space in systems with broken time reversal[1, 51, 52, 56] or inversion symmetry[46, 57] or both[6].

The appearance of Weyl points is governed by the geometry of the band structure and symmetries of the Hamiltonian and lattice. As such, it is possible to observe bosonic analogs of Weyl points. This has already been achieved in artificially designed photonic[9, 22, 23, 50] and phononic crystals[10, 55], and proposed for magnons[21, 33, 37–39, 48]. Quantum magnets are particularly promising since they have for long been a versatile platform to realise complex quantum states of matter including bosonic analogs of novel fermionic phases. The wide range of available quantum magnets with different lattice geometries and the ability to tune their properties readily by external magnetic field make them ideal testbed for realising bosonic analogs of topological states of matter[3, 4, 7, 8, 13, 14, 16–18, 21, 26, 27, 33, 35, 37–40, 43, 44, 48, 58]. However, despite theoretical predictions, experimental observation of Weyl magnons have remained elusive. In this work, we present evidence for the existence of Weyl triplons in the geometrically frustrated Shastry Sutherland compound, $\text{SrCu}_2(\text{BO}_3)_2$. In contrast to previous studies that considered idealized Hamil-

tonians based on families of quantum magnets[33, 37–39], we focus on a realistic microscopic Hamiltonian of the extensively studied geometrically frustrated quantum magnet, $\text{SrCu}_2(\text{BO}_3)_2$ [25, 32, 41]. In this work, we have used experimentally determined Hamiltonian parameters[34] for the microscopic model that have been demonstrated to reproduce faithfully the experimentally observed behavior of the material[32].

II. RESULTS

Microscopic model.

FIG. 1: **The $\text{SrCu}_2(\text{BO}_3)_2$ lattice.** (a) The 3D-schematic lattice structure of compound $\text{SrCu}_2(\text{BO}_3)_2$. The red-bonds are dimer-A and blue-bonds are dimer-B. The green dotted-lines are the inter-layer bonds. (b) The intralayer Heisenberg and DM interactions. (c) The interlayer DM-interactions. (d) The effective square lattice structure after bond-operator transformation.

The figure Fig.1(a) illustrates the three dimensional arrangements of Cu-atoms of $\text{SrCu}_2(\text{BO}_3)_2$ as a coupled layers of Shastry-Sutherland lattice. The Hamiltonian of the system is given by,

$$\begin{aligned}
\mathcal{H} = & J \sum_{\langle i,j \rangle, l} \mathbf{S}_{i,l} \cdot \mathbf{S}_{j,l} + J' \sum_{\langle\langle i,j \rangle\rangle} \mathbf{S}_{i,l} \cdot \mathbf{S}_{j,l} \\
& + \mathbf{D} \cdot \sum_{\langle i,j \rangle, l} (\mathbf{S}_{i,l} \times \mathbf{S}_{j,l}) + \mathbf{D}' \cdot \sum_{\langle\langle i,j \rangle\rangle, l} (\mathbf{S}_{i,l} \times \mathbf{S}_{j,l}) \\
& - B \sum_{i,l} \mathbf{S}_{i,l}^z + J_z \sum_{\substack{i,j \\ \langle l,l' \rangle}} \mathbf{S}_{i,l} \cdot \mathbf{S}_{j,l'} + \mathbf{D}_z \cdot \sum_{\substack{i,j \\ \langle l,l' \rangle}} (\mathbf{S}_{i,l} \times \mathbf{S}_{j,l'}) ,
\end{aligned} \tag{1}$$

where, $\langle i,j \rangle$ and $\langle\langle i,j \rangle\rangle$ denote the summation over the sites belonging to intra-dimer and inter-dimer, bonds respectively in each layer and $\langle l,l' \rangle$ denotes pairs of adjacent layers. The first four terms describe the intra-layer coupling terms and are depicted in Fig.1(b), where J and J' are the intra-dimer and inter-dimer Heisenberg terms. $\mathbf{D}$ and $\mathbf{D}'$ denote the intra-dimer and inter-dimer Dzyaloshinskii–Moriya(DM)-interaction. Finally, J_z and D_z are the inter-layer Heisenberg terms and DM-interactions along the green dotted bonds in Fig.1(a). The fifth term is a Zeeman coupling of the spins with a magnetic field perpendicular to the Shastry-Sutherland layer. We include DM-interactions that are symmetry allowed for $\text{SrCu}_2(\text{BO}_3)_2$ at temperatures below 395K[41, 45, 47] in its low-symmetry phase. In-plane components of the inter-layer DM-interaction is neglected, even though it is allowed by the symmetry of the lattice, since it does not contribute to the low energy physics of the magnetic system. The 2D Hamiltonian describing the magnetic properties of each layer have been extensively studied in the past and the nature of triplon excitations above dimerized ground state and their topological characters delineated using the bond operator formalism[25, 32, 41]. We study the system with additional physically reliable interlayer Heisenberg and DM-interaction terms are included in the Hamiltonian. The interlayer DM-interaction shown in Fig.1(c), is taken in the z-direction and also symmetry allowed by the low temperature crystal-symmetry of $\text{SrCu}_2(\text{BO}_3)_2$. For simplicity, we assume $D_{z2} \approx D_{z1} = D_z$. The presence of interlayer DM-interaction drives a variety of topological phases in the system.

Triplon picture.

The ground state is a product of singlet-dimer states on the red and blue-bonds(Fig.1(a)) in a pure Shastry-Sutherland lattice. A singlet state is a entangled state of two spins such that the wave-function is defined by $|s\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$. The lowest excitations above the ground states are direct product of triplets, which are $|t_x\rangle = i(|\uparrow\uparrow\rangle - |\downarrow\downarrow\rangle)/\sqrt{2}$, $|t_y\rangle = (|\uparrow\uparrow\rangle + |\downarrow\downarrow\rangle)/\sqrt{2}$, $|t_z\rangle = -i(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$. In presence of the small perturbative DM-interaction the ground state is the product state of the rotated-singlets $|\tilde{s}_A\rangle$ and $|\tilde{s}_B\rangle$. The rotated singlets and rotated triplets are related to the original singlet and triplets, as written below,

$$\begin{pmatrix} |\tilde{s}_A\rangle \\ |\tilde{t}_A^x\rangle \\ |\tilde{t}_A^y\rangle \\ |\tilde{t}_A^z\rangle \end{pmatrix} = \begin{pmatrix} 1 & -\alpha & 0 & 0 \\ \alpha & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} |s_A\rangle \\ |t_A^x\rangle \\ |t_A^y\rangle \\ |t_A^z\rangle \end{pmatrix}, \tag{2}$$

$$\begin{pmatrix} |\tilde{s}_B\rangle \\ |\tilde{t}_B^x\rangle \\ |\tilde{t}_B^y\rangle \\ |\tilde{t}_B^z\rangle \end{pmatrix} = \begin{pmatrix} 1 & 0 & \alpha & 0 \\ 0 & 1 & 0 & 0 \\ -\alpha & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} |s_B\rangle \\ |t_B^x\rangle \\ |t_B^y\rangle \\ |t_B^z\rangle \end{pmatrix}, \tag{3}$$

where, $\alpha = \frac{|D|}{2J}$. To study the low temperature excitation above the ground state, we used bond operator formalism[41, 42], which is the ideal formalism to treat a dimerized system in a mean field level. In this formalism, we consider the product state of singlets as the vacuum-state and we treat triplets as the quasi-particle excitations named as triplon. The triplon quasi-particles hop around the effective square lattice consisting of two different sub-lattices as shown in Fig.1(d). The low energy effective Hamiltonian in terms of triplons, is further transformed using unitary transformation, such that the two sub-lattices of the effective squared lattice become equivalent. The real-space triplon-Hamiltonian after neglecting the terms of order of α^2 is given by,

$$\begin{aligned}
\mathcal{H} = & J \sum_{\mathbf{r}_i} \sum_{\mu=x,y} \hat{t}_{\mathbf{r}_i}^{\mu\dagger} \hat{t}_{\mathbf{r}_i}^{\mu} + i h_z \sum_{\mathbf{r}_i} [\hat{t}_{\mathbf{r}_i}^{x\dagger} \hat{t}_{\mathbf{r}_i}^y - \hat{t}_{\mathbf{r}_i}^{y\dagger} \hat{t}_{\mathbf{r}_i}^x] \\
& - \frac{i D'_{\perp}}{2} \sum_{\mathbf{r}_i} \sum_{\alpha=x,y} [\hat{t}_{\mathbf{r}_i+\delta_{\alpha}}^{y\dagger} \hat{t}_{\mathbf{r}_i}^x + \hat{t}_{\mathbf{r}_i}^{y\dagger} \hat{t}_{\mathbf{r}_i+\delta_{\alpha}}^x - \text{h.c.}] \\
& + \frac{i \tilde{D}'_{||,s}}{2} \sum_{\mathbf{r}_i} [+ \hat{t}_{\mathbf{r}_i+\delta_x}^{z\dagger} \hat{t}_{\mathbf{r}_i}^y + \hat{t}_{\mathbf{r}_i+\delta_x}^{y\dagger} \hat{t}_{\mathbf{r}_i}^z - \text{h.c.} \\
& \quad - \hat{t}_{\mathbf{r}_i+\delta_y}^{z\dagger} \hat{t}_{\mathbf{r}_i}^x - \hat{t}_{\mathbf{r}_i+\delta_y}^{x\dagger} \hat{t}_{\mathbf{r}_i}^z - \text{h.c.}] \\
& - i D_z \sum_{\mathbf{r}_i} [\hat{t}_{\mathbf{r}_i+\delta_z}^{y\dagger} \hat{t}_{\mathbf{r}_i}^x + \hat{t}_{\mathbf{r}_i}^{y\dagger} \hat{t}_{\mathbf{r}_i+\delta_z}^x - \text{h.c.}] .
\end{aligned} \tag{4}$$

The coupling terms J_z and $D'_{||,ns}$ do effects the energy of order of magnitude less than α^2 . Again the term $\tilde{D}'_{||,s}$ consists the interaction terms $D'_{||,s}$ and D , such that $\tilde{D}'_{||,s} = D'_{||,s} - \frac{|D|J'}{2J}$. The interplay between the DM-interactions D_z and $D'_{\perp}$ generates different kinds of Weyl-triplons in the system. In the following sub-section, we discuss about the momentum space Hamiltonian and the topological Weyl-triplons in the system.

Topological Weyl-triplons.

The momentum space triplon-Hamiltonian is given as,

$$\mathcal{H} = \sum_{\mathbf{k}} \sum_{\mu,\nu=x,y,z} \hat{t}_{\mu,\mathbf{k}}^{\dagger} M_{\mu\nu}(\mathbf{k}) \hat{t}_{\nu,\mathbf{k}}, \tag{5}$$

where the matrix $M(\mathbf{k})$ is given by,

$$M(\mathbf{k}) = \begin{pmatrix} J & ig_z h_z + 2iD'_\perp \gamma_3 & \tilde{D}'_{||} \gamma_2 \\ -ig_z h_z - 2iD'_\perp \gamma_3 & J & -\tilde{D}'_{||} \gamma_1 \\ \tilde{D}'_{||} \gamma_2 & -\tilde{D}'_{||} \gamma_1 & J \end{pmatrix} \quad (6)$$

where, $\gamma_1 = \sin(k_x)$, $\gamma_2 = \sin(k_y)$, $\gamma_3 = \frac{1}{2}(\cos(k_x) + \cos(k_y))$, $\gamma_4 = \cos(k_z)$. We study the model fixing the parameters $J = 722$ GHz, $|\tilde{D}'_{||}| = 20$ GHz, $D'_\perp = -21$ GHz and $g_z = 2.28$ [34, 41] and varying the parameters h_z and D_z . At a fixed $\mathbf{k}$ -point in momentum space the matrix Eq.6 has three eigen-values, J , $J + \frac{|d(\mathbf{k})|}{2}$ and

$J - \frac{|d(\mathbf{k})|}{2}$. Thus at low energies, the system has three different triplon bands and the possible points at which the band-crossing happens are the high-symmetry points on the k_x - k_y plane, which are $(\pi, 0)$, $(0, \pi)$, $(0, 0)$, (π, π) . The Weyl-points at the high symmetry points are triply degenerate, which has no equivalence in the high energy physics, because the quasi-particle excitation triplons in this system do not follow the Poincare symmetry[5, 36].

The schematic figure of different types of Weyl-points in the Brillouin-zone(BZ) is shown in Fig.2(a). The red-dots illustrates the Weyl-points at positions $(0, \pi, k_{z1})$ and $(\pi, 0, k_{z1})$, where $k_{z1} = \cos^{-1}\left(-\frac{h_z g_z}{2D_z}\right)$. The blue dots denote the Weyl-points at position $(0, 0, k_{z2})$, where $k_{z2} = \cos^{-1}\left(-\frac{h_z g_z + 2D'_\perp}{2D_z}\right)$. Again, the green-points are Weyl-points at position (π, π, k_{z3}) , where $k_{z3} = \cos^{-1}\left(\frac{2D'_\perp - h_z g_z}{2D_z}\right)$.

FIG. 2: **Weyl triplons in Brillouin Zone(BZ).** (a) A schematic picture for the presence of possible Weyl-points. The color coding is further described in the main text. The Weyl-points in BZ for parameters (b) $D_z = D'_\perp/2$, $h_z = 0$, (c) $D_z = D'_\perp/2$, $h_z = h_c$, (d) $D_z = D'_\perp$, $h_z = h_c/2$, (e) $D_z = 3D'_\perp$, $h_z = 0$, (f) $D_z = 3D'_\perp$, $h_z = 0$. Where, $h_c = \frac{2D'_\perp}{g_z}$. The blue arrows illustrate the direction of the Berry-curvature. The red curves show the change in the Chern number of the lowest band due to the Weyl-points.

To verify the band closing points are Weyl-points, we plot the direction of Berry curvature and change in Chern-number within the first-BZ in Fig.2(b)-(f), for different parameter regions. It is noted that the Chern number changes by ± 2 for the Weyl-points present at $(0, 0, \pm k_{z2})$ and $(\pi, \pi, \pm k_{z3})$ and so the monopole charge associated with these Weyl-points are ± 2 . Moreover, the Chern-number changes by ± 4 and it is due to the joint contributions of the Weyl-points at $(0, \pi, \pm k_{z1})$ and $(\pi, 0, \pm k_{z1})$,

each of which carries a monopole charge of ± 2 .

FIG. 3: **Topological Phase diagram.** The color coded region of topological phase diagram is defined based on the number of Weyl-points and based on the position of the Weyl-points in the BZ. The subdivision of the regions (a), (b), (c), (d) denotes the qualitative changes in the Weyl-points. Further description is provided in the main text.

parameter space in to several coloured regions in Fig.3. The region-I and region-II are the regions without Weyl-points, but in region-II the bands are topological whereas the bands in region-I, are trivial in Chern number. The Chern-number of upper band and lower-band are ± 2 for a fixed k_z -value and the middle band is flat with zero Chern number. For $D_z = 0$, the phase transition from region-I to region-II happens at critical magnetic field $h_c = \frac{2|D_z|}{g_z}$ [41].

The nature of Weyl-points in the residual regions III, IV, V and VI depend on the sign of the DM-interaction $D'_\perp$. Here we describe the phase diagram for $D'_\perp < 0$. The region-III consists of two pairs of Weyl-points at positions $(0, \pi, \pm k_{z1})$ and $(\pi, 0, \pm k_{z1})$ as in Fig.2(b). The region-IV contains one-pair of Weyl-points $(0, 0, \pm k_{z2})$ as in Fig.2(c). Moreover, the region-V includes three-pairs of Weyl-points at $(0, \pi, \pm k_{z1})$, $(\pi, 0, \pm k_{z1})$ and $(0, 0, \pm k_{z2})$ as in Fig.2(d). The region-VI consists of four-pairs of Weyl-points at $(\pi, \pi, \pm k_{z3})$, $(0, \pi, \pm k_{z1})$, $(\pi, 0, \pm k_{z1})$ and $(0, 0, \pm k_{z2})$ as in Fig.2(e)-(f). The Weyl-points at different sub-regions (a), (b), (c), (d) are at the same position but, the nature of Weyl-points changes (See Supplementary material). For the case $D'_\perp > 0$, the Weyl-nodes at $(0, 0, \pm k_{z2})$ are substituted by the Weyl-nodes at $(\pi, \pi, \pm k_{z3})$ and vice-versa.

FIG. 4: **Surface magnon-arcs and surface states.** Triplon-arcs on the x - z surface (a), (b), (c), (d) for the parameters same as in (b), (c), (d), (e) in Fig.1. The surface states on the x - z surface for the parameters (e), (f), (g), (h) for the parameters same as in (a), (b), (c), (d) respectively.

Surface arcs and surface states.

The topological nature of the system is revealed by the presence of the surface states in the material. In Fig.4(a)-(d), we plot the surface spectral function of a slab geometry of a system extended along x - z direction. Each of

the projected bulk Weyl-points on the surface emits two triplon-arcs, which divulge that the monopole charge of a Weyl-point is ± 2 . The surface triplon-arcs of the system is quite different in the different regions of parameter space, because of the different position and different numbers of Weyl-points present in different sector in the pa-

parameter phase. The Fig.4(a), (b), (c), (d) illustrates the surface triplon-arcs for the topological phase regime III, IV, V, VI respectively. For illustration, we describe the Fig.4(a), which corresponds to the region-IIIa in phase diagram Fig.3. There are two-pairs of Weyl-triplon in this region, at positions $(0, \pi, \pm k_{z1})$ and $(\pi, 0, \pm k_{z1})$. So the projected Weyl-point on the k_x - k_z surface exists at the positions $(\pi, \pm k_{z1})$ and $(0, \pm k_{z1})$. The pair of points along k_z axis is connected by two surface triplon-arcs. The existence of surface triplon-arcs in the system can be detected using inelastic neutron scattering. The Fig.4(e)-(h), describes that the surface states are chiral gap-less state present within the bulk gap in the system.

Thermal Hall effect for experimental detection.

Thermal Hall effect is the key experimental signature to detect topological excitations in a magnetic system. The characteristic features of Thermal Hall conductance of an Weyl-magnon bands is different from the usual gapped topological magnon bands, making it an ideal probe to detect Weyl points. We calculate the thermal Hall effect in different regimes with Weyl points (phases III, IV, V or VI in Fig.3), gapped topological triplons (phases I, II in Fig.3) and gapped topologically trivial triplon excitations to show that the thermal Hall conductivity exhibits distinct features identifying the different regimes. Since the Weyl-points in this system always occur in pairs aligned along the z -direction, a transverse current cannot be created along the z -axis. Similarly, a temperature gradient along this direction cannot produce a transverse current along any other direction[38]. However, a transverse triplon current can be induced in y (or x)-direction by applying a temperature gradient along the y (or x)-direction. The thermal Hall conductance of the system in the $x - y$ plane is given by[15, 29–31],

$$\kappa_{xy} = \int_{-\pi}^{\pi} \frac{dk_z}{2\pi} \kappa_{xy}^{2D}(k_z), \quad (7)$$

where $\kappa_{xy}^{2D}(k_z)$ is the 2D-thermal Hall conductance contribution from the $k_x - k_y$ -plane of fixed k_z -value in the Brillouin Zone, which is given by,

$$\kappa_{xy}^{2D}(k_z) = -T \int \int \frac{dk_x dk_y}{(2\pi)^2} \sum_{n=1}^N c_2(f^B[E_n(\mathbf{k})]) \Omega_n^z(\mathbf{k}), \quad (8)$$

where, $\mathbf{k} = (k_x, k_y, k_z)$ and $c_2(x) = (1+x)(\ln \frac{1+x}{x})^2 - (\ln x)^2 - 2\text{Li}_2(-x)$, with $\text{Li}_2(x)$ as bilogarithmic function.

FIG. 5: Thermal Hall Conductivity. The thermal Hall conductance as a function of the magnetic field is shown for $D_z = \frac{D'_z}{4}$. As magnetic field increases the system undergoes different phase regions as in Fig.3. The dots are calculated Thermal Hall conductivity and the red-line is analytically fitted with the expressions $A\Delta k_{zi}(h_z) + B$ as discussed in the main text. The inset shows the distance between Weyl-nodes as a function of the magnetic field for phase regions III(a) and V(a) in Fig.3.

While the nature and magnitude of interlayer DM-interaction (D_z) in $\text{SrCu}_2(\text{BO}_3)_2$ has not been determined experimentally, it is reasonable to expect finite D_z as its presence is allowed by symmetry of the lattice. We assume a small, but finite, interlayer DMI parallel to the layers (as allowed by the symmetry of the lattice), such that the triplon bands of the system lies in region III(a) of Fig.3. Assuming $D_z = \frac{D'_z}{4}$ the thermal Hall conductivity is plotted as a function of magnetic field in Fig.5 for $0 \leq h_z \leq 2h_c$. The triplon bands undergo several topological phase transitions in this range of applied field – III(a) $\rightarrow$ II(a) $\rightarrow$ IV(a) $\rightarrow$ I in Fig.3. The triplon bands in region III(a) contains two pairs of Weyl points at $(0, \pi, \pm k_{z1})$ and $(\pi, 0, \pm k_{z1})$, while there is one pair of Weyl points at $(0, 0, \pm k_{z2})$ in the region V(a). The triplon bands are fully gapped and topological in nature in region II(a), whereas they are gapped and topologically trivial in region I. It is noted that, although the Berry curvature at the Weyl point is ill-defined, the thermal Hall conductance $\kappa_{xy}^{2D}(k_z)$ is a continuous function of k_z , because the left and right hand limit $k_z \rightarrow k_{zw} + 0^+$ and the left hand limit as $k_z \rightarrow k_{zw} + 0^-$ are equal, where k_{zw} denotes the position of the Weyl-point. The thermal Hall conductance exhibits a unique quasi-linear dependence as a function of magnetic field for a region with Weyl-points, and quite different from the phase region without Weyl points. This is because the thermal Hall conductance of magnetic excitations (magnons or triplons) is proportional to the distance between the Weyl-nodes in momentum space[38], analogous to that of (electrical) Hall

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conductance observed in Weyl semimetals[59]. In regions III(a) and V(a) the distance between the pair of Weyl-nodes are $\Delta k_{z1}(h_z) = 2 \cos^{-1}(-\frac{h_z g_z}{2D_z})$ and $\Delta k_{z2}(h_z) = 2\pi - 2 \cos^{-1}(-\frac{h_z g_z + 2D'_z}{2D_z})$ respectively. The inset of the Fig.5 shows the distance between the Weyl-nodes as a function of magnetic field has point of inflection at the points $h_z = 0$ and $h_z = h_c$, which gives rise to the quasi-linear behaviour of the thermal Hall conductance. To show the quasi-linear dependence of the thermal Hall conductance in Weyl-triplon region as a function of magnetic field, the thermal conductivity is fitted with the analytical expression $A\Delta k_{zi}(h_z) + B$, where A and B are fitting parameters and $i = 1$ or 2 . The quasi-linear characteristic in thermal Hall conductance in this system is solely due to the presence of the Weyl-nodes. On the other hand, the field dependence of the thermal Hall conductance is markedly different in region $IV(a)$ where the triplon bands are fully gapped and carry finite Chern numbers, consistent with previous studies[25, 41]. Thus the presence of quasi-linearity in the thermal Hall conductance as a function of magnetic field is a direct evidence of the presence of Weyl-nodes. Finally, in region I with topologically trivial, gapped triplon bands, the thermal hall conductivity vanishes.

III. CONCLUSION

In conclusion we have demonstrated that $\text{SrCu}_2(\text{BO}_3)_2$ is a possible host of Weyl-triplons. Our study shows that interlayer perpendicular DM-interaction (even if very small in magnitude) naturally give rise to the Weyl-triplons. Furthermore the nature of triplon bands at low temperature depends neither on the interlayer Heisenberg interaction (because of orthogonal Dimer arrangement) nor on the interlayer in-plane DM-interactions, which makes the appearance of Weyl nodes robust against small deviations from the idealized model. Finally, We have shown that the quasi-linear behaviour of thermal Hall conductance as a function of magnetic field is a possible experimental signature to detect the presence of Weyl nodes. We also propose neutron scattering experiment as an alternative way to explore the Weyl-nodes in the triplon bands. Similar Weyl-triplon phases can also be investigated in the dimer phases of materials $\text{Rb}_2\text{Cu}_3\text{SnF}_{12}$ [12, 28] and $\text{ZnCu}_3(\text{OH})_6\text{Cl}_2$ [49].

DATA AVAILABILITY

The data that support the findings of this study are available from the corresponding author upon reasonable request.

The code that supports the findings of this study are available from the corresponding author upon reasonable request.

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Dhiman Bhowmick and Pinaki Sengupta initiated the project. Dhiman Bhowmick calculated and plotted all the results. All the authors checked the validity of the results and equally contributed to write the manuscript.

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ETHICS DECLARATIONS**Competing interests**

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Figures

Figure 1

The SrCu₂(BO₃)₂ lattice. (a) The 3D schematic lattice structure of compound SrCu₂(BO₃)₂. The red-bonds are dimer-A and blue-bonds are dimer-B. The green dotted-lines are the inter-layer bonds. (b) The intralayer Heisenberg and DM interactions. (c) The interlayer DM-interactions. (d) The effective square lattice structure after bond-operator transformation.

Figure 2

Weyl triplons in Brillouin Zone(BZ). (a) A schematic picture for the presence of possible Weyl-points. The color coding is further described in the main text. The Weyl-points in BZ for parameters (b) $D_z = D_0? = 2$,

$h_z = 0$, (c) $D_z = D_0 = 2$, $h_z = h_c$, (d) $D_z = D_0$, $h_z = h_c = 2$, (e) $D_z = 3D_0$, $h_z = 0$, (f) $D_z = 3D_0$, $h_z = 0$. Where, $h_c = 2D_0 \cdot g_z$. The blue arrows illustrate the direction of the Berry-curvature. The red curves show the change in the Chern number of the lowest band due to the Weyl-points.

Figure 3

Topological Phase diagram. The color coded region of topological phase diagram is defined based on the number of Weyl-points and based on the position of the Weyl-points in the BZ. The subdivision of the regions (a), (b), (c), (d) denotes the qualitative changes in the Weyl-points. Further description is provided in the main text.

Figure 4

Surface magnon-arcs and surface states. Triplon-arcs on the x-z surface (a), (b), (c), (d) for the parameters same as in (b), (c), (d), (e) in Fig.1. The surface states on the x-z surface for the parameters (e), (f), (g), (h) for the parameters same as in (a), (b), (c), (d) respectively.

Figure 5

Thermal Hall Conductivity. The thermal Hall conductance as a function of the magnetic field is shown for $D_z = D_0/4$. As magnetic field increases the system undergoes different phase regions as in Fig.3. The dots are calculated Thermal Hall conductivity and the red-line is analytically fitted with the expressions $A \tan(k_z(h_z)) + B$ as discussed in the main text. The inset shows the distance between Weyl-nodes as a function of the magnetic field for phase regions III(a) and V(a) in Fig.3.

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